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Patentanmeldung Nr. Patent application No. Demande de brevet n°

03023136.9

PRIORITY DOCUMENT
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Im Auftrag

For the President of the European Patent Office

Le Président de l'Office européen des brevets
p.o.

R C van Dijk

Anmeldung Nr:
Application no.: 03023136.9
Demande no:

Anmeldetag:
Date of filing: 10.10.03
Date de dépôt:

Anmelder/Applicant(s)/Demandeur(s):

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Bezeichnung der Erfindung/Title of the invention/Titre de l'invention:
(Falls die Bezeichnung der Erfindung nicht angegeben ist, siehe Beschreibung.
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Crystals of an aurora-a tpx2 complex, tpx2 binding site of aurora-a, aurora-a ligands and their use

In Anspruch genommene Priorität(en) / Priority(ies) claimed /Priorité(s) revendiquée(s)
Staat/Tag/Aktenzeichen/State/Date/File no./Pays/Date/Numéro de dépôt:

Internationale Patentklassifikation/International Patent Classification/
Classification internationale des brevets:

C12N9/00

Am Anmeldetag benannte Vertragstaaten/Contracting states designated at date of filing/Etats contractants désignées lors du dépôt:

AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LU MC NL PT RO SE SI SK TR LI

CRYSTALS OF AN AURORA-A TPX2 COMPLEX, TPX2 BINDING SITE OF AURORA-A, AURORA-A LIGANDS AND THEIR USE

The present invention relates to crystals of phosphorylated Aurora-A kinase fragment alone and in complex with a ligand, amino acid residues 1-43 of human TPX2. This invention also relates to methods for designing and selecting ligands, in particular allosteric inhibitors of Aurora-A, that bind to the Aurora-A kinase and their use. Further, the present invention relates to certain indene and indole derivatives.

At the beginning of mitosis, eukaryotic cells undergo a dramatic reorganization. The nuclear envelope breaks down and microtubules rearrange around chromatin into a bipolar spindle structure that carries out the duty of separating sister chromatids. Chromatin signals to the spindle assembly machinery through Ran, a small Ras-like GTPase that is concentrated in its GTP-bound form around chromatin. Ran function in spindle assembly is connected to its role in nucleocytoplasmic transport . RanGTP releases crucial spindle assembly factors such as TPX2 and NuMA from the transport factors that mediate their import into the nucleus at interphase. After nuclear envelope breakdown, the presence of free TPX2 in the vicinity of chromatin is thought to nucleate microtubules that are subsequently organised into a spindle by microtubule motors. Additionally, TPX2 localises an essential mitotic kinase, Aurora-A, to spindle microtubules (Kufer, T. A., Sillje, H. H., Korner, R., Gruss, O. J., Meraldi, P., and Nigg, E. A. (2002). Human TPX2 is required for targeting Aurora-A kinase to the spindle. J. Cell Biol. *158*, 617-623).

Aurora kinases constitute a family of serine-threonine protein kinases whose localization and activities are precisely choreographed as a cell progresses through mitosis. Aurora-A is a cell-cycle regulated serine-threonine kinase involved in chromosome segregation and cytokinesis (Bischoff, J.R. and Plowman, G.D. (1999). The Aurora/Ipl1p kinase family: regulators of chromosome segregation and cytokinesis. Trends Cell Biol. 9, 454-459). It plays a major role in cell-cycle progression and has also been described as an oncogene. It maps to a chromosome region frequently amplified in tumours (Dutertre, S. et al. (2002). On the role of Aurora A in centrosome function. Oncogene 21, 6175-6183). It is overexpressed in a variety of human tumours, in particular breast and colon cancer, but has limited expression in normal tissues (Sen, S. et al. (1997). A putative serine/threonine kinase encoding gene BTAK on chromosome 20q13 is amplified and overexpressed in human breast cancer cell lines. Oncogene 14, 2195-2200; Bischoff, J.R. et al. (1998). A homologue of Drosophila Aurora kinase is oncogenic and amplified in human colorectal cancers. EMBO J. 17, 3052-3065). Overexpression of active Aurora-A transforms rat fibroblasts so that they

are capable of growing tumours in nude mice, while an inactive mutant is unable to cause oncogenic transformations. As an oncogenic protein kinase, Aurora-A is a target for the development of specific inhibitors that may be useful as cancer therapeutics. Despite the importance of Aurora-A for both cell division and cancer perspectives, little is known at present about its downstream targets and activation/deactivation mechanisms.

Several factors contribute to the activity of a serine/threonine kinase. These include the proper positioning of active site residues and the correct organisation of the substrate-binding site (the "activation segment"). Phosphorylation of a threonine residue within the activation segment is often required to elicit kinase activity and Aurora-A is no exception. Phosphorylation of a threonine in the Aurora-A activation segment ($Thr288^{AUR}$, human numbering) is crucial for activity, although it is unclear as to whether it is catalysed *in vivo* by an upstream kinase or by Aurora-A itself (Bischoff, et al. (1999) *supra*). Structural studies of c-AMP dependent protein kinase (cAPK) have shown that when the corresponding threonine residue ($Thr197^{cAPK}$) is phosphorylated, the activation segment is in an active conformation. Cyclin-dependent kinases (CDKs) require not only phosphorylation of the equivalent threonine ($Thr160^{CDK}$) but also the binding by a partner protein, cyclin-A, to be fully activated. Aurora-A might also rely on a similar mechanism. It has recently been reported that in vertebrates the interaction of Aurora-A with a partner protein, TPX2, leads to a strong activation of the kinase. Upon TPX2 binding, the *in vitro* autophosphorylation activity of Aurora-A is increased and dephosphorylation is prevented (Kufer et al., (2002) *supra*).

ATP competitive inhibitors that are specific for different kinases are used as therapeutic agents in cancer treatment (Garcia-Echeverria, C., et al. (2000). ATP site-directed competitive and irreversible inhibitors of protein kinases. Med. Res. Rev. 20, 28-57). Although ATP-binding sites at the moment are the most common targets for the design of kinase inhibitors, it is difficult to achieve selectivity of such inhibitors due to the similarity in kinase active sites, which only have minor differences of surrounding amino-acid residues (Cheetham, G.M.T. et al. (2002). Crystal structure of Aurora-2, an oncogenic serine-threonine kinase. J. Biol. Chem. 277, 42419-42422).

The structure of unphosphorylated Aurora-A has been previously reported (Cheetham, G.M.T. et al. (2002). Crystal structure of Aurora-2, an oncogenic serine-threonine kinase. J. Biol. Chem. 277, 42419-42422; Nowakowski, J. et al. (2002). Structures of the cancer-related Aurora-A, FAK, and EphA2 protein kinases from nanovolume crystallography. Structure 10, 1659-1667). Aurora-A has the typical three-dimensional structure of protein kinases, with the active site situated between the N- and C-terminal lobe. Binding of ATP

involves amino-acid residues that are conserved among all kinases. Extensive structural work has shown that kinases in their active state all assume a similar structural framework, with the 'activation segment' in a similar conformation competent for substrate binding (Huse, M. and Kuriyan, J. (2002). The conformational plasticity of protein kinases. Cell 109, 275-282). However, they differ in the molecular mechanisms to achieve such an active form. In the case of Abl kinase, subtle differences in its activation mechanisms have been exploited with the development of the Abl-specific inhibitor Gleevec, which is used as a leukaemia therapeutic agent (Capdeville, R. et al. (2002). Glivec (STI571, imatinib), a rationally developed, targeted anticancer drug. Nat. Rev. Drug Discov. 1, 493-502).

In the case of Aurora-A, activation is achieved by both phosphorylation and by the binding of a specific activator, the protein TPX2 (Eyers, P.A., et al. (2003). A novel mechanism for activation of the protein kinase Aurora-A. Curr. Biol. 13, 691-697). Blocking this activator-binding site would provide a means to downregulate this kinase specifically.

In view thereof, it was an object of the present invention to elucidate the structure of the Aurora-A TPX2 binding site, to provide means for identifying compounds that bind to Aurora-A and preferably modulate Aurora-A activity, and to provide such compounds.

The present invention relates to (a) crystals of a fragment of phosphorylated human Aurora-A kinase alone (amino acid residues 122-403; hereinafter referred to as Aurora-A(ΔN)), and (b) crystals of said fragment of phosphorylated human Aurora-A kinase in complex with a ligand, i. e. an Aurora-A ligand complex. The Aurora-A ligand is a fragment of TPX2 which is a minimal activating domain of TPX2. The minimal activating domain of TPX2 consists of amino acid residues 1-43 of human TPX2 and hereinafter is referred to as TPX2(1-43).

The present invention provides the structure coordinates of the phosphorylated human Aurora-A(ΔN) kinase. The complete coordinates are listed in Table A.

The present invention also provides the structure coordinates of the phosphorylated human Aurora-A(ΔN)/TPX2(1-43) complex. The complete coordinates are listed in Table B.

The present invention also describes a method for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which contain at least some structurally similar features to the Aurora-A TPX2 binding domain. It is preferred that these molecules or molecular complexes comprise at least a part of the ligand binding site defined by structure coordinates of Aurora-A amino acids Q127, W128, R126, L159, F157,

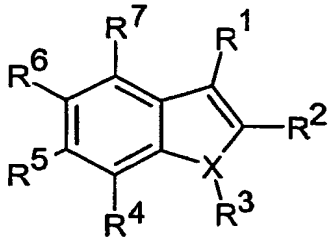
E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 according to Table B, or a mutant or homologue thereof. The numbering system as used herein refers to the protein sequences for human Aurora-A.

The present invention also provides a machine-readable data storage medium which comprises a data storage material encoded with machine readable data defined by the structure coordinates of phosphorylated human Aurora-A(ΔN) kinase according to Table A or a homologue thereof, or of the phosphorylated human Aurora-A(ΔN)/TPX2(1-43) complex according to Table B.

The present invention further provides a binding site in Aurora-A for an Aurora-A ligand such as TPX2 or fragments thereof, as well as methods for designing or selecting further Aurora-A ligands and in particular Aurora-A modulators including agonists, partial agonists, antagonists, partial antagonists of Aurora-A using information about the crystal structures disclosed herein.

The present invention further provides allosteric inhibitors of Aurora-A, wherein at least a portion of the inhibitor binds with any portion or all of residues Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A according to Table B.

The present invention in particular relates to indole and indene derivatives of formula (I)



(I)

wherein

R^1 represents hydrogen, alkylene-NHR^8, alkylene-OR^8, or alkylene-SR^8;

R^2 represents hydrogen, alkylene-NHR^8, alkylene-OR^8, or alkylene-SR^8;

R^3 represents hydrogen, alkyl, alkylene-R^9, alkenylene-R^9, alkynylene-R^9, or arylene-R^9;

R^4 represents hydrogen;

R^5 represents hydrogen, alkyl, OR^{10}, NHR^{10}, SR^{10}, alkylene-R^{10}, alkenylene-R^{10}, alkynylene-R^{10}, or arylene-R^{10};

R^6 represents hydrogen, alkyl, OR^{10}, NHR^{10}, SR^{10}, alkylene-R^{10}, alkenylene-R^{10}, alkynylene-R^{10}, or arylene-R^{10};

R^7 represents hydrogen;
R^8 represents hydrogen, CO-alkyl, $(aa)_m asp(aa)_n$, $(aa)_m glu(aa)_n$, or $(aa)_m cys(aa)_n$;
R^9 represents NH-alkyl, $N(alkyl)_2$, $N^+(alkyl)_3$, aryl, or heteroaryl;
R^{10} represents hydrogen, aryl, or substituted aryl;
X represents a nitrogen atom or CH;
aa represents an amino acid residue; and
n is zero or an integer of 1 to 10;
m is zero or an integer of 1 to 10,
provided that R^1 and R^2 are not both hydrogen and that R^5 and R^6 are not both hydrogen, and optical isomers, physiologically acceptable salts and prodrugs thereof.

The present invention also relates to the pharmaceutical compostions containing Aurora-A ligands, such as said indole and indene derivatives, and the use of Aurora-A ligands, such as said indole and indene derivatives, in therapy, in particular in cancer treatment.

In the drawings the figures show as

(figure 1) (A) anti-*Xenopus* TPX2 Western blot (upper panel) and anti-*Xenopus* Aurora-A Western blot (lower panel) of GST (glutathione S transferase) (lanes 1 and 2), GST *Xenopus* TPX2 (lanes 3 and 4) or GST *Xenopus* TPX2(1-39) (lanes 5 and 6) which proteins were incubated in *Xenopus* cytostatic factor (CSF) arrested extracts in the presence or absence of RanQ69L-GTP and immunoprecipitated with GST antibody-coated beads;
(B) anti-GST Western blot (upper panel) and anti-human Aurora-A Western blot (lower panel) of GST (lane 1), GST TPX2(1-43) (lane 2) or GST TPX2(15-43) (lane 3) proteins that were incubated in mitotic HeLa cell extract and immunoprecipitated with GST antibody-coated beads;
(C) autoradiography of the SDS-PAGE gel (left panel) and the corresponding Coomassie-stained gel (right panel) after *in vitro* phosphorylation (γ^{32}P-ATP) of histone H3 by human Aurora-A in the presence of full-length TPX2, GST TPX2(1-43) or GST TPX2(15-43) (lanes 2, 3 and 4 respectively);
(D) much of the phosphorylation signal in GST after *in vitro* phosphorylation (γ^{32}P-ATP) of TPX2(1-43) by Aurora-A (lane 1) followed by TEV cleavage (lane 2);
(E) an anti-human Aurora-A Western blot (upper panel) and an anti-phosphoAurora-A Western blot (lower panel) after phosphatase PP1 treatment of human Aurora-A in the absence or presence of full-length TPX2,

GST TPX2(1-43) or GST TPX2(15-43) followed by detection of Aurora-A by a polyclonal antibody (upper panel) and an antibody specific for Aurora-A phosphorylated at Thr288^{AUR} (lower panel);

(figure 2) (A) an *in vitro* pull-down assay with respect to the binding of full-length Aurora-A, AuroraΔN or AuroraΔN(D274N) to GST TPX2(1-43) (lanes 4, 5 and 6), and to GST (lanes 1, 2 and 3);

(B) an anti-phospho Aurora-A Western blot of wild-type Aurora(ΔN) and the D274N mutant when expressed in *E. coli.*

(C) autoradiograph for detecting i*n vitro* phosphorylation of histone H3 by Aurora(ΔN) in the presence or absense of TPX2(1-43) (lane 2 compared to lane 1), the cleaved (lane 2) or uncleaved (lane 3) GST TPX2(1-43) fusion protein;

(D) Sequence alignment of TPX2 N-terminal domain from human (*H*), *Xenopus* (*X*) and puffer fish (*F*), secondary structure elements being shown above the sequences *in red* (upstream extended stretch) and *pink* (downstream helical stretch), and intervening residues not modelled being marked with a dotted line;

(E) Sequence alignment of Aurora-A kinase catalytic domain from three vertebrate species that contain TPX2 (human, *H.AUR-A*; *Xenopus*, *X.AUR-A*; puffer fish, *F AUR-A*), two invertebrates that do not contain TPX2 (*Drosophila, D.AUR-A; C.elegans, C.AUR-A*) together with human and *Xenopus* Aurora-B (*H.AUR-B*, *X.AUR-B*) and vertebrate cAPK, wherein Aurora-A secondary structural elements are labelled above the alignment, the phosphorylated Thr288 (human numbering) is shown, and residues that interact with 7-21^{TPX} or 30-43^{TPX} being indicated by filled or open circles respectively;

(figure 3) ribbon style drawings of the structure of Aurora-A bound to TPX2 as

(A) a view of the complex between the catalytic domain of human Aurora (AuroraΔN) and the N-terminal domain of TPX2 shown in typical kinase orientation, an upstream stretch of TPX2 binding at the N-terminal lobe of Aurora-A, and a downstream stretch binding between the two lobes, and a dotted line marking the approximate path of the linker connecting the two TPX2 stretches (disordered and not modelled);

(B) a view of the complex after a 180° rotation about the vertical axis in respect to view in panel A showing more clearly the two stretches of TPX2 that bind to Aurora-A;

(C) the upstream stretch of TPX2 (residues 7-21^{TPX}) that binds at a hydrophobic surface groove present in the N-terminal lobe of the kinase,

wherein details of the extensive interactions are shown in the same orientation as in panel B;

(D) the downstream helical stretch of TPX2 (residues 30-43^{TPX}) that binds Aurora-A near helix αC and the activation segment, close to but not directly in contact with phospho-Thr288^{AUR}, wherein details of interactions being shown in the same orientation as in panel B and C.

(figure 4) ribbon style drawings of conformational states of phosphorylated Aurora-A in the presence and absence of TPX2 as

(A) an overlay showing that the structures of Aurora-A when bound to TPX2 and when unbound are closely superposable at the position of active site residues and of helix αC, but diverge at the activation segment between residues His280^{AUR} and Leu293^{AUR}, wherein Phospho-Thr288^{AUR} points inwards in the TPX2-bound structure and outwards in the kinase alone structure;

(B) an illustration of conformational changes upon TPX2 binding, according to which the activation segments of the kinase alone structure (left panel) and of the TPX2-bound structure (right panel) are shown in a view rotated by approximately 90° with respect to panels A-C, and TPX2 binding results in the reorganization of the activation segment, with a 10 Å movement of Thr288^{AUR};

(C) a schematic representation of the molecular mechanism of TPX2-mediated activation of Aurora-A, according to which the upstream stretch of TPX2 anchors the regulator to the N-terminal lobe of the kinase and the downstream stretch (helix) hooks the activation segment triggering a lever-arm like movement, where rotations at His280^{AUR} and Pro282^{AUR} pull on Thr288^{AUR}.

Using X-ray crystallography, crystal structures of phosphorylated human Aurora-A(ΔN) alone at 2.75 Å resolution and in complex with a minimal activating domain of TPX2 at 2.5 Å resolution have been determined and the specific site of TPX2-mediated activation of Aurora-A has been found. TPX2 binds at two sites on the kinase. One stretch of TPX2 (residues 8-19) binds at the N-terminal lobe of the kinase and another stretch (31-38) binds between the two lobes at the phosphorylated activation segment, positioning it for substrate binding. The TPX2-binding site located on the N-terminal lobe of the kinase consists of an extended surface groove formed by Aurora-specific residues. The groove consists of two pockets, one shaped by residues E170, L169, V206, R179, L178, V182, Y199 and the other shaped by residues Q127, W128, R126, L159 and F157. The two pockets are occupied by hydrophobic side chains of TPX2, Y8, Y10, A12 and P13 on one side, and F16, I17 and F19

on the other. From the structure and biochemical data it is concluded that binding of this TPX2 stretch is necessary but not sufficient for activation of Aurora-A, allowing the downstream TPX2 stretch to bind with enough affinity to achieve activation. Binding of a small-molecule inhibitor to the TPX2-recognition groove on the N-terminal lobe of Aurora-A *would* decrease the activity of this kinase by blocking its specific activation mechanism.

The Aurora-A kinase and the TPX2 protein described herein are intended to include any polypeptide which has the activity of the naturally occurring Aurora-A kinase and TPX2 protein, respectively. Aurora-A and TPX2 contemplated herein include all vertebrate and mammalian forms such as rat, mouse, pig, goat, horse, guinea pig, rabbit, monkey, orangutan and human. Such terms also include polypeptides that differ from naturally occurring forms of Aurora-A kinase and TPX2 protein by having amino acid deletions, substitutions, and additions, but which retain the activity of Aurora-A kinase and TPX2 protein, respectively. Particular Aurora-A sequences are shown in figure 2E and particular TPX2 sequences are shown in figure 2D. According to the present invention, the human sequences are preferred.

The crystal structures of the invention preferably contains at least 25%, more preferably at least 50%, more preferably at least 75%, more preferably at least 90%, more preferably at least 95%, more preferably at least 99%, and most preferably all of the coordinates listed in Table A and Table B, respectively.

The crystal of the phosphorylated human Aurora-A(ΔN) kinase of the invention preferably has the following unit cell dimensions in angstroms: a = 81.18 ± 5%, b = 81.18 ± 5%, c = 169.62 ± 5% and the space group $P6_122$.

The crystal of the phosphorylated human Aurora-A(ΔN) kinase/TPX2(1-43) complex of the invention preferably has the following unit cell dimensions in angstroms: a = 59.63 ± 5%, b = 81.72 ± 5%, c = 70.38 ± 5% and an orthorhombic space group $P2_12_12_1$.

The three-dimensional structure of the phosphorylated human Aurora-A(ΔN) kinase and of the phosphorylated human Aurora-A(ΔN) kinase/TPX2(1-43) complex of this invention are defined by a set of structure coordinates as set forth in Table A and Table B, respectively. The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of the protein or protein complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the

crystal. The electron density maps are then used to establish the positions of the individual atoms of the complex.

Those of skill in the art will understand that a set of structure coordinates for a kinase or a kinase/ligand complex or a fragment thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape.

The variations in coordinates discussed above may be generated because of mathematical manipulations of the structure coordinates. For example, the structure coordinates set forth in Table A could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates; integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same.

Various computational analyses are therefore necessary to determine whether a molecule or molecular complex or a portion thereof is sufficiently similar to all or parts of the kinase or the kinase/ligand complex described above as to be considered the same. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA) version 4.1, and as described in the accompanying User's Guide.

The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in Molecular Similarity to compare structures is divided into four steps: 1) load the structures to be compared; 2) define the atom equivalences in these structures; 3) perform a fitting operation; and 4) analyze the results.

Each structure is identified by a name. One structure is identified as the target (i. e., the fixed structure); all remaining structures are working structures (i. e., moving structures). Since

atom equivalency within QUANTA is defined by user input, for the purpose of this invention we will define equivalent atoms as protein backbone atoms (N, C and O) for all conserved residues between the two structures being compared. We will also consider only rigid fitting operations.

When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by QUANTA.

For the purpose of this invention, any molecule or molecular complex that has a root mean square deviation of conserved residue backbone atoms (N, C, O) of less than 1.5 A when superimposed on the relevant backbone atoms described by structure coordinates listed in Table A or Table B are considered identical. More preferably, the root mean square deviation is less than 1.0 A. In a preferred embodiment of the present invention, the molecule or molecular complex comprises at least a portion of the ligand binding site defined by structure coordinates of Aurora-A amino acids Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 according to Table B, or a mutant or homologue of said molecule or molecular complex. More preferred are molecules or molecular complexes comprising all or any part of the ligand binding site defined by structure coordinates of Aurora-A amino acids Y199, L178, W128, H187, L188, I184 according to Table B, or a mutant or homologue of said molecule or molecular complex.

The term "complex" or "molecular complex" means Aurora-A or a mutant or homologue of Aurora-A in a covalent or non-covalent association with a chemical entity or compound.

For purposes of the present invention, by "at least a portion of" it is meant all or any part of the ligand binding site defined by these structure coordinates.

By "mutant or homologue" as used herein it is meant a molecule or molecular complex having a similar structure and/or sequences to Aurora-A or TPX2. By "similar structure" it is meant a mutant or homologue having a binding pocket or binding domain that have a root mean square deviation from the backbone atoms of said Aurora-A or TPX2 amino acids of not more than 1.5 Angstroms. By "similar sequence" it is meant a mutant or homologue having 30%, or more preferably 75%, identity with Aurora-A or TPX2 over an amino acid

sequnce of at least 30, preferably at least 50, in particular at least 100 and especially at least 200 consecutive amino acid.

The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a protein or protein complex from the relevant portion of the backbone of the Aurora-A fragment of the complex as defined by the structure coordinates described herein.

Once the structure coordinates of a protein crystal have been determined they are useful in solving the structures of other crystals.

Thus, in accordance with the present invention, the structure coordinates of the kinase ot the kinase/ligand complex, and portions thereof is stored in a machine-readable storage medium. Such data may be used for a variety of purposes, such as drug discovery and x-ray crystallographic analysis of protein crystals.

Accordingly, in one embodiment of this invention is provided a machine-readable data storage medium comprising a data storage material encoded with the structure coordinates set forth in Table A and/or with the structure coordinates set forth in Table B.

For the first time, the present invention permits the use of structure-based or rational drug design techniques to design, select, and synthesize chemical entities, including inhibitory and stimulatory compounds that are capable of binding to Aurora-A, or any portion thereof.

One particularly useful drug design technique enabled by this invention is iterative drug design. Iterative drug design is a method for optimizing associations between a protein and a compound by determining and evaluating the three-dimensional structures of successive sets of protein/compound complexes.

Those of skill in the art will realize that association of natural ligands or substrates with the binding pockets of their corresponding kinases or enzymes is the basis of many biological mechanisms of action. The term "binding pocket" as used herein, refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity or compound. Similarly, many drugs exert their biological effects through association with the binding pockets of kinases and enzymes. Such associations

may occur with all or any parts of the binding pockets. An understanding of such associations will help lead to the design of drugs having more favorable associations with their target kinase, and thus, improved biological effects. Therefore, this information is valuable in designing potential ligands or inhibitors of Aurora-A kinase.

The term "associating with" refers to a condition of proximity between chemical entities or compounds, or portions thereof. The association may be non-covalent--wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions--or it may be covalent.

In iterative drug design, crystals of a series of protein/compound complexes are obtained and then the three-dimensional structures of each complex is solved. Such an approach provides insight into the association between the proteins and compounds of each complex. This is accomplished by selecting compounds with inhibitory activity, obtaining crystals of this new protein/compound complex, solving the three-dimensional structure of the complex, and comparing the associations between the new protein/compound complex and previously solved protein/compound complexes. By observing how changes in the compound affected the protein/compound associations, these associations may be optimized.

In some cases, iterative drug design is carried out by forming successive protein-compound complexes and then crystallizing each new complex. Alternatively, a pre-formed protein crystal is soaked in the presence of a compound, thereby forming a protein/compound complex and obviating the need to crystallize each individual protein/compound complex.

As used herein, the term "soaked" refers to a process in which the crystal is transferred to a solution containing the compound of interest.

The structure coordinates set forth in Table A and Table B can also be used to aid in obtaining structural information about another crystallized molecule or molecular complex. This may be achieved by any of a number of well-known techniques, including molecular replacement.

The structure coordinates set forth in Table A and Table B can also be used for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which contain at least some structurally similar features to Aurora-A. In particular, structural information about another crystallized molecule or molecular complex may be obtained. This

may be achieved by any of a number of well-known techniques, including molecular replacement.

Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a crystallized molecular complex whose structure is unknown comprising the steps of:

a) generating an X-ray diffraction pattern from said crystallized molecular complex;

b) applying at least a portion of the structure coordinates set forth in Table A and Table B to the X-ray diffraction pattern to generate a three-dimensional electron density map of the molecular complex whose structure is unknown; and

c) using all or a portion of the structure coordinates set forth in Table A and Table B to generate homology models of Aurora-A or any other kinase ligand binding domain.

Preferably, the crystallized molecular complex is obtained by soaking a crystal of this invention in a solution.

By using molecular replacement, all or part of the structure coordinates of the Aurora-A ligand complex provided by this invention or molecular complex whose structure is unknown more quickly and efficiently than attempting to determine such information ab initio.

Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases for the unknown structure.

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the Aurora-A ligand complex according to Table B within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model

building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex [E. Lattman,"Use of the Rotation and Translation Functions", in Meth. Enzymol., 115, pp. 55-77 (1985); M. G. Rossmann, ed.,"The Molecular Replacement Method", Int. Sci. Rev. Set., No. 13, Gordon & Breach, New York (1972)].

The structure of any portion of any crystallized molecule or molecular complex, or mutant, or homologue that is sufficiently homologous to any portion of the Aurora-A ligand complex can be solved by this method.

The structure coordinates are also particularly useful to solve the structure of crystals of Aurora-A ligand co-complexed with a variety of chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including interaction of candidate Aurora-A inhibitors with the complex. For example, high resolution X-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to these sites can then be designed and synthesized and tested for their Aurora-A inhibition activity.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.5-3 A resolution X-ray data to an R value of about 0.20 or less using computer software, such as X-PLOR [Yale University, 1992, distributed by Molecular Simulations, Inc.; see, e. g., Blundell & Johnson, supra; Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)]. This information may thus be used to optimize Aurora-A agonists, partial agonists, antagonists, partial antagonists, and more importantly, to design new Aurora-A agonists/antagonists.

Accordingly, the present invention is also directed to a binding site in Aurora-A for an Aurora-A ligand in which a portion of Aurora-A ligand is in van der Walls contact or hydrogen bonding contact with at least one of the following residues: Y199, L178, W128, L159, H187, L188, I184 of Aurora-A.

For purposes of this invention, by Aurora-A binding site it is also meant to include mutants or homologues thereof. In a preferred embodiment, the mutants or homologues have at least 25% identity, more preferably 50% identity, more preferably 75% identity, and most preferably 95% identity to residues Q127, W128, R126, L159, F157, E170, L169, V206,

Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A binding sites.

The present invention is also directed to a machine-readable data storage medium, comprising a data storage material encoded with machine readable data, wherein the data is defined by the structure coordinates of an Aurora-A ligand complex according to Table B or a homologue of said complex, wherein said homologue comprises backbone atoms that have a root mean square deviation from the backbone atoms of the complex of not more than 3.0 Å preferably of not more that 2.0 Å.

The present invention also provides for computational methods using three-dimensional models of the Aurora-A kinase that are based on crystals of the kinase or the kinase ligand complex. Generally, the computational method of designing an Aurora-A ligand determines which amino acid or amino acids of Aurora-A interact with a chemical moiety (at lease one) of the ligand using a three-dimensional model of a crystallized protein comprising the Aurora-A kinase with a bound ligand and selecting a chemical modification (at least one) of the chemical moiety to produce a second chemical moiety with a structure that either decreases or increases an interaction between the interacting amino acid and the second chemical moiety compared to the interaction between the interacting amino acid and the corresponding chemical moiety on the natural ligand, i.e. TPX2 or a fragment thereof.

The computational methods of the present invention are for designing kinase synthetic ligands using such crystal and three dimensional structural information to generate synthetic ligands that modulate the conformational changes of the kinase. These computational methods are particularly useful in designing an agonist, partial agonist, antagonist or partial antagonist to the kinase, wherein the agonist, partial agonist, antagonist or partial antagonist has an extended moiety that prevents any one of a number of ligand-induced molecular events that alter the kinase's influence on one of its targets, such as preventing the normal coordination of the activation domain observed for a naturally occurring ligand or other ligands that mimic the naturally occurring ligand, such as an agonist. As described herein, synthetic ligands of the kinase will be useful in modulating kinase activity in a variety of medical conditions.

Aurora-A is known to comprise various segments as follows: 1) an amino-terminal ligand-binding site; and 2) an Aurora-A activation segement.

This modularity permits different segments and sites of each protein to separately accomplish different functions, although the segments and sites influence each other.

Exploiting the TPX2-binding site in the N-terminal lobe of Aurora-A has the advantage of blocking the activation of this oncogenic kinase and of blocking it specifically. An Aurora-A specific inhibitor would be an important cancer therapeutic agent in particular for breast and colon tumours.

The polypeptides referred to herein (e. g., Aurora-A, TPX2, and the like) may be produced by any well-known method, including synthetic methods, such as solid phase, liquid phase and combination solid phase/liquid phase syntheses; recombinant DNA methods, including cDNA cloning, optionally combined with site directed mutagenesis; and/or purification of the natural products, optionally combined with enzymatic cleavage methods to produce fragments of naturally occurring forms of Aurora-A and TPX2. The peptides can be expressed, crystallized, its three dimensional structure determined with a ligand bound (either using crystal data from the same kinase or a different kinase or a combination thereof), and computational methods used to design ligands to its ligand binding site, particularly ligands that contain an extension moiety that coordinates the activation segment of Aurora-A.

Typically Aurora-A and TPX2 as well as fragments thereof are purified to homogeneity for crystallization.

Purity of Aurora-A is measured with SDS-PAGE, mass spectrometry and hydrophobic HPLC. The purified Aurora-A for crystallization should be at least 97.5 % pure or 97.5%, preferably at least 99.0% pure or 99.0% pure, more preferably at least 99.5% pure or 99.5% pure.

Initially purification of the unliganded kinase can be obtained by conventional techniques, such as size exclusion chromatography, hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC), and heparin affinity chromatography.

To achieve higher purification for improved crystals of Aurora-A, it will be desirable to ligand shift purify the kinase using a column that separates the kinase according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted kinase with a ligand, especially an agonist or partial agonist. The ligand induces a change in the kinase's surface charge such that when rechromatographed on the same column, the kinase then

elutes at the position of the liganded kinase are removed by the original column run with the unliganded kinase. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the column.

More recently developed methods involve engineering a "tag" such as with histidine placed on the end of the protein, such as on the amino terminus, and then using a nickle chelation column for purification, Janknecht R., Proc. Natl. Acad. Sci. USA Vol 88: 8972-8976 (1991) incorporated by reference.

Typically, purified Aurora-A is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be stablished between 2 and 37 °C, although the kinase tends to be more stable in the 2-20 °C range.

Preferably crystals are made with the hanging and/or sittiing drop methods.

Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25 °C are generally used and it is often preferable to test crystallization over a range of temperatures. It is preferable to use crystallization temperatures from 18 to 25 °C, more preferably 20 to 23 °C, and most preferably 22 °C.

The Aurora-A ligand of this invention is any peptide, peptide mimetic or nonpeptide, including small organic molecules, that is capable of acting as a ligand for Aurora-A. In a preferred embodiment, the Aurora-A ligand is an Aurora-A modulator. By" Aurora-A modulator " it is meant an agonist or activator, a partial agonist or partial activator, an antagonist or inhibitor, or a partial antagonist or partial inhibitor of the Aurora-A kinase.

Agonists or partial agonists induce changes in kinases that place them in an active conformation that allows them to influence one of its targets. There may be several different ligand-induced changes in the kinase's conformation.

Antagonists or partial antagonists bind to kinases, but fail to induce conformational changes that alter the kinase's target-influencing properties or physiologically telcram conformations. Binding of an antagonist or partial antagonist can also block the binding and therefore the actions of an agonist or partial agonist.

Partial agonists, or partial antagonists, bind to kinases and induce only part of the changes in the kinases that are induced by agonists or antagonists, respectively. The differences can

be qualitative or quantitative. Thus, a partial agonist or partial antagonist may induce some of the conformation changes induced by agonists or antagonists, respectively, but not others, or it may only induce certain changes to a limited extent.

As described herein, the unliganded kinase is in a configuration that is either inactive, has some activity or has phosphorylating activity. Binding of agonist ligands induces conformational changes in the kinase such that the kinase becomes more active and/or is protected from deactivation, in particular from dephosphorylation.

According to a particular embodiment, the present invention relates to allosteric inhibitors of Aurora-A. The binding of such an allosteric inhibitor to Aurora-A results in a conformational change of the kinase, thereby decreasing the kinases's activity, preferably by blocking its activation mechanism. The preferred binding site of an allosteric inhibitor according to the present invention is the TPX2-recognition groove where TPX2 binds Aurora-A, as described herein.

Consequently, an extended chemical moiety (or more) from the ligand that stabilizes the binding or contact of the TPX2 binding site with the binding site of Aurora-A can be designed. Typically such chemical moieties will extend past and away from the molecular recognition domain on the ligand and usually past the buried binding cavity of the ligand.

Ligand binding by the kinase is a dynamic process, which regulates kinase function by inducing an altered conformation.

The three-dimensional structure of the liganded Aurora-A kinase can be used in the development of new Aurora-A synthetic ligands. In addition, Aurora-A is overall well suited to modern methods including three-dimensional structure elucidation and combinatorial chemistry such as those disclosed in EP 335 628, U. S. patent 5,463,564, which are incorporated herein by reference. Computer programs that use crystallography data when practicing the present invention enable the rational design of ligands to Aurora-A. Programs such as RASMOL can be used with the atomic coordinates from crystals generated by practicing the invention or used to practice the invention by generating three dimensional models and/or determining the structures involved in ligand binding. Computer programs such as INSIGHT and GRASP allow for further manipulation and the ability to introduce new structures. In addition, high throughput binding and bioactivity assays can be devised using purified recombinant protein and modern assays described herein and known in the art in order to refine the structure of a ligand and thereby the activity.

Generally the computational method of designing an Aurora-A synthetic ligand comprises two steps:

1) determining which amino acid or amino acids of Aurora-A interacts with a first chemical moiety (at least one) of the ligand using a three dimensional model of a crystallized protein comprising Aurora-A with a bound ligand; and

2) selecting chemical modifications (at least one) of the first chemical moiety to produce a second chemical moiety with a structure to either decrease or increase an interaction between the interacting amino acid and the second chemical moiety compared to the interaction between the interacting amino acid and the first chemical moiety.

Preferably the method is carried out wherein said three dimensional model is generated by comparing isomorphous ligand derivatives to produce improved phasing. Further preferred is wherein said method comprises determining a change in interaction between said interacting amino acid and said ligand after chemical modification of said first chemical moiety, especially wherein said three dimensional model is generated by comparing isomorphous ligand derivatives to produce improved phasing. Also preferred is wherein said selecting uses said first chemical moiety that interacts with at least one of the interacting amino acids Y199, L178, W128, L159, H187, L188, I184.

As shown herein, interacting amino acids form contacts with the ligand and the center of the atoms of the interacting amino acids are usually 2 to 4 angstroms away from the center of the atoms of the ligand. Generally these distances are determined by computer, however distances can be determined manually once the three dimensional model is made. See also Wagner et al., Nature 378 (6558): 670-697 (1995) for stereochemical figures of-three dimensional models. More commonly, the atoms of the ligand and the atoms of interacting amino acids are 3 to 4 angstroms apart. The invention can be practiced by repeating steps I and 2 to refine the fit of the ligand to the ligand bindiung site and to determine a better ligand, such as an agonist, partial agonist, antagonist or partial antagonist.

The three dimensional model of Aurora-A can be represented in two dimensions to determine which amino acids contact the ligand and to select a position on the ligand for chemical modification and changing the interaction with a particular amino acid compared to that before chemical modification. The chemical modification may be made using a computer, manually using a two dimensional representation of the three dimensional model or by chemically synthesizing the ligand. The ligand can also interact with distant amino

acids after chemical modification of the ligand to create a new ligand. Distant amino acids are generally not in contact with the ligand before chemical modification. A chemical modification can change the structure of the ligand to make as new ligand that interacts with a distant amino acid usually at least 4.5 angstroms away from the ligand, preferably wherein said first chemical moiety is 6 to 12 angstroms away from a distant amino acid. Often distant amino acids will not line the surface of the binding cavity for the ligand, they are too far away from the ligand to be part of a pocket or binding cavity. The interaction between an amino acid of the ligand binding site and an atom of a ligand can be made by any force or attraction described in nature. Usually the interaction between the atom of the amino acid and the ligand will be the result of a hydrogen bonding interaction, charge interaction, hydrophobic interaction, van der Waals interaction or dipole interaction. In the case of the hydrophobic interaction it is recognized that this is not a per se interaction between the amino acid and ligand, but rather the usual result, in part, of the repulsion of water or other hydrophilic group from a hydrophobic surface. Reducing or enhancing the interaction of the ligand binding site and a ligand can be measured by calculating or testing binding energies, computationally or using thermodynamic or kinetic methods as known in the art.

Chemical modifications will often enhance or reduce interactions of an atom of an amino acid of the ligand binding site and an atom of a ligand. Steric hindrance will be a common means of changing the interaction of the ligand binding cavity with the activation segment.

The present invention also provides methods for identifying compounds that modulate kinase activity. Various methods or combinations thereof can be used to identify these compounds. For example, test compounds can be modeled that fit spatially into the Aurora-A ligand binding site as defined by structure coordinates according to Table B, or using a three-dimensional structural model of Aurora-A, mutant Aurora-A or Aurora-A homolog or portion thereof. Structure coordinates of the ligand binding site, in particular amino acids Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 can also be used to identify structural and chemical features. Identified structural or chemical features can then be employed to design or select compounds as potential Aurora-A modulators. By structural and chemical features it is meant to include, but is not limited to, van der Waals interactions, hydrogen bonding interactions, charge interaction, hydrophobic bonding interaction, hydrophobic interaction and dipole interaction. Alternatively, or in conjunction, the three-dimensional structural model or the ligand binding site can be employed to design or select compounds as potential Aurora-A modulators. Compounds identified as potential Aurora-A modulators can then be

synthesized and screened in an assay characterized by binding of a test compound to the Aurora-A.

Examples of assays useful in screening of potential Aurora-A modulators include, but are not limited to, screening in silico, in vitro assays and high throughput assays, for instance, based on phosphorylation of histone H3 as described herein (Crosio, C., Fimia, G. M., Loury, R., Kimura, M., Okano, Y., Zhou, H., Sen, S., Allis, C. D., and Sassone-Corsi, P. (2002). Mitotic phosphorylation of Histone H3: spatio-temporal regulation by mammalian Aurora kinases. Mol. Cell Biol. 22, 874-885).

A preferred method of the invention can be described as a computational method of designing an kinase antagonist from an kinase agonist comprising:

1) determining a structure of a molecular recognition site of said agonist using a three dimensional model of a crystallized protein comprising an Aurora-A, and
2) selecting at least one chemical modification of said agonist that provides a ligand structure that extends beyond a binding site for said agonist and in the direction of at least one protein site important in Aurora-A biological function.

Another preferred method of the invention can be described as a computational method of designing a selective kinase modulator such as an kinase super agonist or antagonist comprising:

1) determining at least one interacting amino acid of an Aurora-A that interacts with at least one first chemical moiety of said ligand using a three dimensional model of a crystallized protein comprising Aurora-A with a bound ligand, and
2) selecting at least one chemical modification of said first chemical moiety to produce a second chemical moiety with a structure to reduce or enhance an interaction between said

interacting amino acid and said second chemical moiety compared to said interaction between said interacting amino acid and said first chemical moiety.

However, as will be understood by those of skill in the art upon this disclosure, other structure based design methods can be used. Various computational structure based design methods have been disclosed in the art.

For example, a number computer modeling systems are available in which the sequence of the Aurora-A and the Aurora-A structure (i. e., atomic coordinates of Aurora-A and/or the atomic coordinates of the active site, the bond and dihedral angles, and distances between

atoms in the active site such as provided in Table A and Table B) can be input. This computer system then generates the structural details of the site in which a potential Aurora-A modulator binds so that complementary structural details of the potential modulators can be determined. Design in these modeling systems is generally based upon the compound being capable of physically and structurally associating with Aurora-A. In addition, the compound must be able to assume a conformation that allows it to associate with Aurora-A. Some modeling systems estimate the potential inhibitory or binding effect of a potential Aurora-A modulator prior to actual synthesis and testing.

Methods for screening chemical entities or fragments for their ability to associate with Aurora-A are also well known. Often these methods begin by visual inspection of the active site on the computer screen. Selected fragments or chemical entities are then positioned with the Aurora-A. Docking is accomplished using software such as QUANTA and SYBYL, following by energy minimization and molecular dynamics with standard molecular mechanic forcefields such as CHARMM and AMBER. Examples of computer programs which assist in the selection of chemical fragment or chemical entities useful in the present invention include, but are not limited to, GRID (Goodford, P. J. J. Med. Chem.1985 28: 849-857), AUTODOCK (Goodsell, D. S. and Olsen, A. J. Proteins, Structure, Functions, and Genetics 1990 8: 195-202), and DOCK (Kunts et al. J. Mol. Biol. 1982 161: 269-288).

Upon selection of preferred chemical entities or fragments, their relationship to each other and Aurora-A can be visualized and the entities or fragments can be assembled into a single potential modulator.

Programs useful in assembling the individual chemical entities include, but are not limited to CAVEAT (Bartlett et al. Molecular Recognition in Chemical and Biological Problems Special Publication, Royal Chem. Soc. 78,182-196 (1989)) and 3D Database systems (Martin, Y. C. J. Med. Chem. 1992 35: 2145-2154).

Alternatively, compounds may be designed de novo using either an empty active site or optionally including some portion of a known inhibitor. Methods of this type of design include, but are not limited to LUDI (Bohm H-J, J. Comp. Aid. Molec. Design 1992 6: 61-78) and LeapFrog (Tripos Associates, St. Louis. MO).

Examples of preferred ligands include the above-described indole and indene derivatives of formula (I), and optical isomers, physiologically acceptable salts and prodrugs thereof.

The physiologically acceptable salts in the present case can be acid addition or base addition salts.

For acid addition salts, inorganic acids, such as hydrochloric acid, sulphuric acid, nitric acid or phosphoric acid, or organic acids, in particular carboxylic acids, e.g. acetic acid, tartaric acid, lactic acid, citric acid, malic acid, mandelic acid, ascorbic acid, maleic acid, fumaric acid, gluconic acid or sulphonic acids, e.g. methanesulphonic acid, benzenesulphonic acid and toluenesulphonic acid, and the like are used.

The base addition salts include salts of the compounds of the formula (I) with inorganic bases, such as sodium hydroxide or potassium hydroxide, or with organic bases, such as mono-, di- or triethanolamine.

Prodrugs of the compounds of the formula I are, for example, physiologically easily hydrolysable esters such as alkyl, pivaloyloxymethyl, acetoxymethyl, phthalidyl, indenyl and methoxymethyl esters.

If the compounds according to the invention have asymmetric centres, racemates and optical isomers are included as mixtures or in pure form (enantiomers, diastereomers).

The term "alkyl" includes straight-chain or branched alkyl groups, such as CH_3, C_2H_5, n-propyl, $CH(CH_3)_2$, n-butyl, $CH(CH_3)$-C_2H_5, isobutyl, $C(CH_3)_3$, n-pentyl or n-hexyl, in particular CH_3, C_2H_5 or $CH(CH_3)_2$, preferably having - if not stated otherwise - 1 to 8, in particular 1 to 6 and particularly preferred 1 to 4 carbon atoms.

The term "alkylene" includes straight-chain or branched alkylene groups, such as methylene and ethylene, preferably having - if not stated otherwise - 1 to 8, in particular 1 to 6 and particularly preferrred 1 to 4 carbon atoms.

The term "alkenylene" includes straight-chain or branched, mono- or polyunsaturated alkylene groups, such as ethenylene, preferably having - if not stated otherwise - 2 to 8, in particular 2 to 6 and particularly preferably 2 to 4, carbon atoms.

The term "alkynylene" includes straight-chain or branched, mono- or polyunsaturated alkylene groups, such as ethynylene, preferably having - if not stated otherwise - 2 to 8, in particular 2 to 6 and particularly preferably 2 to 4, carbon atoms.

"Aryl" is in particular a mono- or bicyclic aromatic radical, preferably having 5 to 14 carbon atoms and especially represents naphthyl, indenyl, and in particular phenyl.

"Heteroaryl" is in particular a mono- or bicyclic heteroaromatic radical preferably having 5 to 14 ring atoms and containing 1, 2 or 3 heteroatom(s) independently selected from the group consisting of O, N and S. According to a particular embodiment, bicyclic radicals contain a 5- or 6-membered heteroaromatic radical which is benzo-fused. Heteroaryl includes nitrogen-containing radicals, such as pyrrolyl, imidazolyl, pyrazolyl, pyridazinyl, pyrazinyl, indolyl, quinolinyl, especially pyridyl, pyrimidyl and isoquinolinyl; radicals which contain an oxygen atom or a sulphur atom, such as thienyl, benzothienyl, furanyl and especially benzofuranyl; radicals which contain two or more different heteroatoms, such as thiazolyl, isothiazolyl, thiadiazolyl, isoxazolyl and oxazolyl. Preferred aromatic heterocyclic radicals are, pyridyl and indolyl.

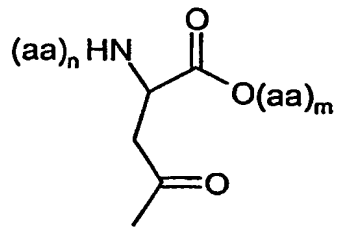
The term "arylene" is preferably naphthylene and in particular phenylene, such as 1,4-phenylene.

According to a preferred embodiment, one of residues R^1 and R^2, preferably residue R^2, is hydrogen while the other, preferably R^1, has a meaning different from hydrogen. In this context, alkylene radicals preferably contain a relatively short main chain connecting the indole or indene moiety with the amino, oxy or thio moiety (-NHR^8, -OR^8 or -SR^8, respectively). Accordingly, the main chain of preferred alkylene radicals contain 1 to 3 carbon atoms. Said alkylene radicals may be branched. Linear alkylene radicals are preferred. Specific examples of alkylene radicals include methylene, eth-1,1-ylene, prop-1,1-ylene and prop-2,2-ylene, with methylene being preferred.

According to a particularly preferred embodiment, one of residues R^1 and R^2, preferably R^2, is hydrogen and the other, preferably R^1, represents alkylene-NHR^8.

R^8 preferably represents an acyl radical so as to form an amide, ester or thioester bond within residue R^1 and/or R^2. It is preferred that residue R^8 represents an amino acid selected from the group consisting of aspartate (asp), glutamate (glu), and cysteine (cys), i.e., n and m are zero, or a peptide connected via aspartate, glutamate or cysteine, i.e., aa represents an amino acid radical, and at least one of n and m is an integer of 1 or higher, wherein the amino acid radicals can be the same or different. The aspartate, glutamate and cysteine radicals may be bonded to the alkylene radical via any of their functional groups. The aspartate and glutamate radicals are preferably bonded via any of its carboxy groups, the β-

carboxy function of aspartate and the γ-carboxy function of glutamate being preferred. Cystein radicals are preferably bonded via their side chain thio functionality. Accordingly, the amino acid radicals aa are connected to the alkylene group via the remaining functional groups of the aspartate, glutamate or cysteine radicals. According to a preferred embodiment, the remaining functional groups are the α-amino group and the α-carboxy group, of which one or both can be bonded to the amino acid radicals aa. According to this embodiment, the connecting aspartate, glutamate or cystein radical is itself part of the peptide chain which is connected to the alkylene residue via the side chain of said aspartate, glutamate or cystein radical. A specific example of such a preferred residue R^8 is a radical of the formula (II)



(II)

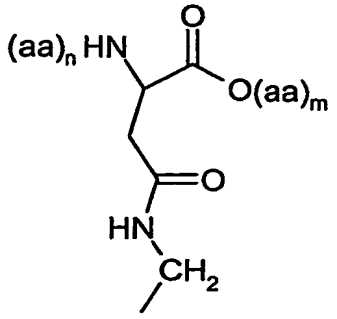
wherein

aa represents an amino acid radical;

n is zero or an integer of 1 to 10; and

m is zero or an integer of 1 to 10.

A specific example of such preferred residues R1 and/or R2 is thus the radical of formula (III)



(III)

wherein

aa represents an amino acid radical;

n is zero or an integer of 1 to 10; and

m is zero or an integer of 1 to 10.

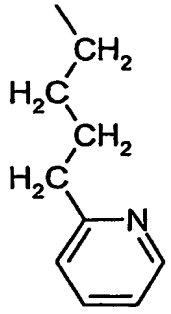
The amino acid radicals aa may be any amino acid. Preferably said amino acid radicals are selected to mimick – together with the connecting amino acid - a portion of TPX2 that binds to Aurora-A. Said portion of TPX2 is in particular a portion comprising the amino acid

sequence from residues 7 to 21, preferably 8 to 19 (compare Fig. 3C) or a fragment thereof. Accordingly, suitable peptides may have the sequence Tyr-Xaa1-Tyr-Xaa2-Ala-Pro-Xaa3-Xaa4-Phe-Xaa5-Xaa6-Phe or a portion thereof, wherein Xaa1-6 may be any amino acid radical. Xaa1 preferably is a serine radical or a similar amino acid. Xaa2 preferably is an aspartate radical or a similar amino acid. Xaa3 preferably is a serine radical or a similar amino acid. Xaa4 preferably is an aspartate radical or a similar amino acid. Xaa5 preferably is an isoleucine radical or a similar amino acid. Xaa6 preferably is an asparagine radical or a similar amino acid. A particularly preferred portion is the sequence Tyr-Xaa1-Tyr-Xaa2-Ala-Pro-Xaa3-Xaa4-Phe. By similar amino acid is meant an amino acid that is considered to result in a conservative change of the peptide's structure when it replaces the amino acid to which it is similar. For instance, aspartate is similar to glutamate. The peptide preferably has a lenght of 3 to 15, more preferably of 4 to 10 and advantagously of 5 to 8 amino acid, the sum of n + m thus being 2 to 14, more preferably of 3 to 9 and advantagously of 4 to 7, respectively.

R^3 preferably is a radical different from hydrogen and advantageously represents alkylene-R^9, alkenylene-R^9, or alkynylene-R^9. In this context, the main chain connecting the indene or indole moiety with residue R^9 preferably is relatively long. Accordingly, it is preferred that the main chain of the alkylene radical, alkenylene radical or alkynylene radical contains 3 to 8, e.g. 4, carbon atoms. Said alkylene radical, alkenylene radical and alkynylene radical may be branched. Linear radicals are preferred. Specific examples of said radicals include prop-1,3-ylene, but-1,4-ylene, pent-1,5-ylene and hex-1,6-ylene, with but-1,4-ylene being preferred.

R^9 preferably represents aryl or heteroaryl. Specific examples of aryl and heteroaryl radicals include phenyl, naphthyl, indenyl, pyridyl, and indolyl, with pyridyl, e.g. pyrid-2-yl, being preferred.

A specific example of such a preferred residue R^3 is a radical of the formula (IV)



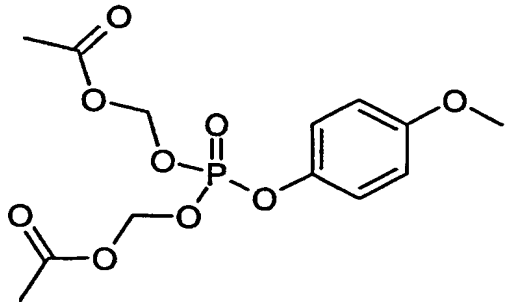
(IV)

While residues R^4, R^5, R^6 and R^7 all may be hydrogen, it is preferred that at least one of said residues, especially R^6, is different from hydrogen.

R^5 and/or R^6 preferably represent OR^{10}, NHR^{10}, SR^{10}, or alkylene-R^{10}. In this context, the preferred embodiments regarding the alkylene radical are those as described in connection with residues R^1 and R^2.

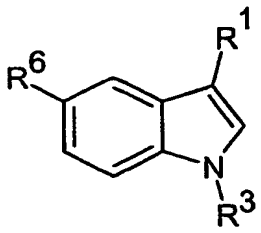
R^{10} preferably represents aryl or substituted aryl. In this context, aryl is preferably phenyl. Substituted aryl, in general, contains 1, 2 or 3 substituents which may be the same or different, mono-substitution being preferred. The substituents are preferably selected from the group consisting of hydroxy, $-OPO_3H_2$, $-CH_2PO_3H_2$, $-CF_2PO_3H_2$, -COOH, $-CH(COOH)_2$, $-OPO_3(R^{11})_2$, $-CH_2OPO_3(R^{11})_2$, $-CF_2PO_3(R^{11})_2$, $-COOR^{11}$, and $-CH(COOR^{11})_2$, wherein R^{11} is a radical that is cleavable *in vivo*, converting the carboxylic acid esters, phosphate and phosphonate esters to carboxylates, phosphates or phosphonates, respectively. Suitable examples of R^{11} residues are alkyl, CH_2OCO-alkyl, and C_2H_4-S-CO-alkyl. Especially preferred substituents are selected from the group consisting of $-OPO_3H_2$, $-CH_2PO_3H_2$, $-CF_2PO_3H_2$, $-OPO_3(R^{11})_2$, $-CH_2OPO_3(R^{11})_2$, and $-CF_2PO_3(R^{11})_2$,. A preferred example of a R^{11} residue is $-CH_2OCO$-alkyl, alkyl being linear or branched and having 1 to 6 carbon atoms, e.g. methyl.

A specific example of such preferred residues R5 and/or R6 is the radical of formula (V)



(V)

According to a specific embodiment, the present invention relates to indole derivatives of formula (Ia)



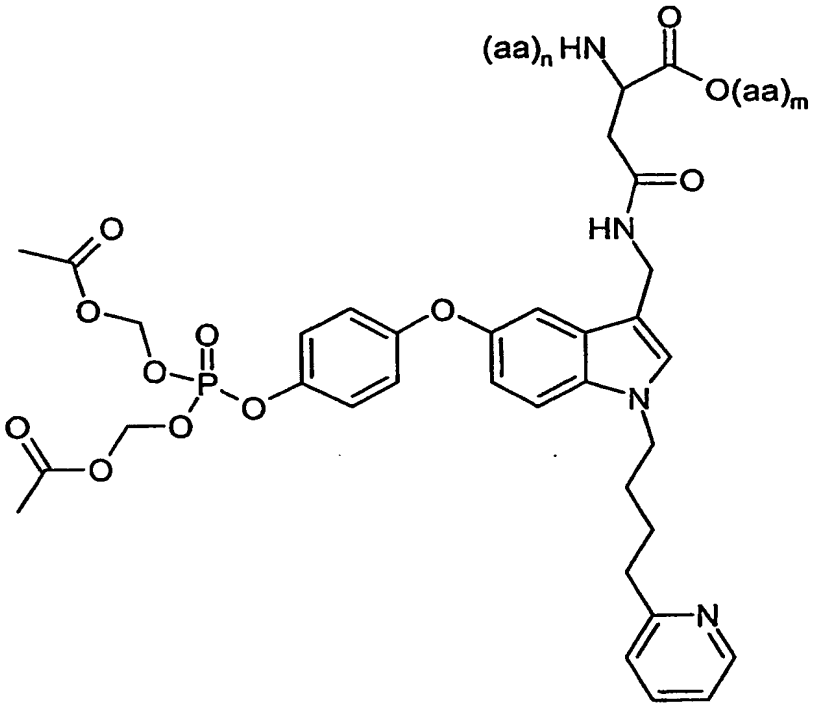
(Ia)

wherein

R^1, R^3 and R^6 are defined as above,

and optical isomers, physiologically acceptable salts and prodrugs thereof.

A preferred indole derivative of the present invention has the formula (1)



1

wherein

aa, n and m are defined as above.

The indene and indole derivatives of formula (I) can be prepared by methods well-known to those skilled in the art.

The present invention is further directed to a method for treating cancer, in particular breast and colon carcinomas, comprising administering an effective amount of an Aurora-A

modulator, such as the indole and indene derivatives as described herein, preferably an antagonist or partial antagonist, identified by a computational process of the invention.

The compounds according to the invention are thus suitable for the treatment of disorders in which the interaction of Aurora-A with TPX2 is responsible for the formation or the progressive course of these disorders. In particular, the compounds according to the invention can be used for the treatment of cancer.

The compounds according to the invention can either be administered as individual therapeutic active compounds or as mixtures with other therapeutic active compounds: they can be administered as such, but in general they are administered in the form of pharmaceutical compositions, i.e. as mixtures of the active compounds with pharmaceutically acceptable excipients, in particular vehicles or diluents and/or additives. The compounds or compositions can be administered enterally, e.g. orally or rectally, or parenterally, e.g. subcutaneously, intravenously or intramuscularly.

The nature of the pharmaceutical composition and of the pharmaceutical carrier or diluent depends on the desired manner of administration. Oral compositions can be present, for example, as tablets or capsules and can contain customary excipients, such as binding agents (e.g. syrup, acacia, gelatin, sorbitol, tragacanth or polyvinylpyrrolidone), fillers (e.g. lactose, sugar, maize starch, calcium phosphate, sorbitol or glycine), lubricants (e.g. magnesium stearate, talc, polyethylene glycol or silica), disintegrating agents (e.g. starch) or wetting agents (e.g. sodium laurylsulphate). Oral liquid preparations can be present in the form of aqueous or oily suspensions, solutions, emulsions, syrups, elixirs or sprays etc. or can be present as dry powders for reconstitution with water or another suitable carrier. Liquid preparations of this type can contain customary additives, for example suspending agents, flavourings, diluents or emulsifiers. For parenteral administration, solutions or suspensions with customary pharmaceutical carriers can be employed.

The following examples are to illustrate the invention, but should not be interpreted as a limitation thereon.

Examples

Experimental Procedures

Protein and Antibody Preparation

AuroraΔN was cloned in pET M11 (residues 122-403, wild-type and D274N) were expressed in CodonPlus RIL *E.coli* (Stratagene) and purified with TALON resin (Clontech) using manufacturer's instructions. AuroraΔN was treated with TEV protease to remove the His tag, passed through a TALON column to remove TEV and then purified to homogeneity by size exclusion chromatography. Human and *Xenopus* GST TPX2 fragments were expressed in BL21(DE3) *E.coli*. TPX2 proteins were purified using glutathione sepharose (Pharmacia). To form the AuroraΔN-TPX2 complex, cell lysate from *E.coli* expressing GST TPX2 was passed through a glutathione sepharose column, washed, and then purified AuroraΔN was passed through the same column. Column resin was incubated with TEV protease to elute the complex, which was further purified by size exclusion chromatography.

The polyclonal antibody against full-length TPX2 was produced in rabbits with bacterially expressed GST TPX2 (Wittmann et al., 2000) and affinity purified. The 1C1 monoclonal anti-*Xenopus* Aurora-A is described in: Giet R, Uzbekov R, Cubizolles F, Le Guellec K, Prigent C., J Biol Chem. (1999) 274, 15005-13. The polyclonal anti-human Aurora-A was obtained by injecting rabbits with bacterially expressed full-length human Aurora-A.

HeLa cell extract and Xenopus egg extract preparation

HeLa cells (CCL2; ATCC, Manassas, VA) were grown in 10% fetal calf serum (FCS) and 2 mM L-glutamine in modified Eagle's medium at 37°C and 5% CO_2. Cells were arrested in S phase using a double thymidine (2 mM) block as described (Stein, 1994) and released from S phase by washing away the thymidine. After 10 h, cells were trypsinized, incubated for 10 min in ice-cold lysis buffer (25 mM Tris pH 7.6, 200 mM NaCl, 1% Triton, protease inhibitors), and centrifuged for 10 min at 15,000 g. *Xenopus* cytostatic factor arrested extracts (CSF extracts) were prepared as described (Murray, 1991).

***In vitro* kinase assay**

Full-length TPX2, TPX2(1-43) or TPX2(15-43) at 4 μM were incubated with full length Aurora-A or AuroraΔN in kinase buffer (20 mM Hepes pH 7.5, 200 mM KCl, 5 mM MgCl2, 0.5 mM EGTA, 1 mM DTT, 0.05 % Triton X-100, 50 μM ATP) containing γ^{32}P-ATP (Amersham) in the presence or absence of histone H3 (0.2 mg/ml, Roche), for 15 min at 25°C. For cleavage, GST TPX2(1-43) was incubated with TEV 16-18h at 4° C (Figure 2C) or by adding TEV after the kinase reaction and incubating 10 min at 30° C (Figure 1D). In Figure 2D, AuroraΔN (8μM) was incubated in kinase buffer containing histone H3 and γ^{32}P-

ATP for 15 min at 25° C. After separation by SDS-PAGE, phosphorylated histone H3 and TPX2 proteins were detected by autoradiography.

Phosphatase assay

Active human Aurora-A (2 μM) was incubated with TPX2, TPX2(1-43) or TPX2(15-43) (3 μM) for 10 min at 4°C. Samples were diluted in phosphatase buffer (50 mM Tris-HCl pH 7, 0.1 mM EDTA, 1 mM $MnCl_2$, 5 mM caffeine, 5 mM DTT, 0.025% Tween 20) and incubated in the absence or presence of PP1 (α isoform, NEB) for 0.5h at 30°C. Afterwards proteins were separated by SDS-PAGE and analyzed by Western blotting with anti-Aurora-A or anti-phospho-Aurora-A (Cell Signalling, 1:10000 dilution).

Immunoprecipitation

For coating beads with anti-GST, 6 μg of antibody were incubated with 20 μl of protein A-conjugated Dynabeads 280 (Dynal) in a total volume of 100 μl PBS-T (PBS, 0.1 % Triton X-100), for at least 1 h at 4°C. The beads were washed twice with PBS-T and twice with HeLa cells lysis buffer or CSF-XB (10 mM Hepes pH 7.7, 50 mM sucrose, 100 mM KCl, 2 mM $MgCl_2$, 0.1 mM $CaCl_2$ and 5 mM EGTA). 50 μl extract was incubated with GST, GST TPX2 1-43, GST TPX2 15-43, GST TPX2 *Xenopus* or GST TPX2(1-39) *Xenopus* proteins (final concentrations: 250 nM *Xenopus*; 1 μM HeLa) in the absence or presence of RanQ69L-GTP (16 μm) for 15 minutes at 20 °C and then added to the beads. After 1 h incubation on ice, the beads were washed twice with lysis buffer or CSF-XB, washed twice with PBS-T and boiled in SDS-PAGE sample buffer. The samples were then subjected to gel electrophoresis and analyzed by Western blotting with anti-GST, anti-*Xenopus* TPX2, anti-*Xenopus* Aurora-A or anti-human Aurora-A.

In vitro pull-down assays

GST or GST TPX2(1-43) (240 μg) was bound to 100 μl glutathione sepharose (Pharmacia) in 1ml binding buffer (PBS, 0.05% Tween-20, 2 mM DTT) for 0.5 h. Beads were washed three times, divided into four equal quantities in 1 ml binding buffer and 35 μg full-length human Aurora-A, AuroraΔN or AuroraΔN(D274N) was added. After binding for 0.5 h at 4°C, the resin was washed four times, then incubated overnight in 50 μl binding buffer plus 2 μg TEV protease. 10 μl supernatant from each was analysed by SDS-PAGE. TEV cleavage was necessary because AuroraΔN and GST TPX 1-43 co-migrate by SDS-PAGE.

Crystallographic methods

Needle-like crystals of AuroraΔN in complex with TPX2 1-43, approximately 10 μm in thickness, were grown at 18°C by vapour diffusion using 18% (w/v) PEG8000, 100 mM MES pH 6.5, 200 mM $MgSO_4$ as well buffer and hanging drops comprising a 1:1 mix of 20 mg/ml complex pre-mixed with 2 mM ATPγS and 0.2 mM $MgSO_4$, and 20% PEG8000, 100 mM MES pH 6.5, 200 mM $MgSO_4$. For cryo-protection, the drop buffer was supplemented with 17.5% (v/v) glycerol. Hexagonal prism crystals of the wild-type AuroraΔN kinase alone, approximately 50μm in all dimensions, were grown by vapour diffusion using 20% PEG300, 5% PEG8000, 100 mM Tris 8.5, 10% glycerol as well buffer and sitting drops comprising a 1:1 mix of well buffer and 9 mg/ml protein pre-incubated with 2 mM ATPγS and 2 mM $MgSO_4$. Diffraction data were collected at 100K and processed using the CCP4 suite of programs (CCP4, 1994). Structures were solved by molecular replacement using CNS (Brunger et al., 1998) and the coordinates of the cAMP-dependent protein kinase catalytic subunit as an initial model (Mashhoon et al., 2001). CNS was used for refinement and O (Jones et al., 1991) for model building. The statistics for data collection and refinement are shown in Table 1. Structure figures were prepared using PyMOL (DeLano, 2002). Coordinates and structure factors have been deposited in the Protein Data Bank with accession codes 1ol7 and 1ol5 for phosphoryated AuroraΔN alone and in complex with TPX2(1-43), respectively.

Mapping of a minimal domain of TPX2 sufficient for binding and activating Aurora-A

A minimal domain of TPX2 sufficient to interact with Aurora-A was mapped. The Aurora-A binding domain of TPX2 resides within its N-terminal 150 residues. Inspection of a sequence alignment of TPX2 shows that only a third of this region is conserved across species (residues 1-43 in human TPX2, 1-39 in *Xenopus* TPX2). This fragment is able to co-immunoprecipitate Aurora-A from *Xenopus* egg extracts to the same extent as the full-length protein (Figure 1A, lanes 6 and 4 respectively). In the egg extracts, efficient binding of TPX2 to Aurora-A requires Ran locked into its GTP-bound form (RanQ69L), which releases TPX2 from a complex with importin α/β. *Xenopus* TPX2(1-39) binds Aurora-A in a RanGTP-independent manner (Figure 1A, lanes 5 and 6), consistent with it lacking the portion of TPX2 regulated by Ran. The corresponding fragment of human TPX2 (residues 1-43) is able to interact with Aurora-A using pull-down experiments in HeLa extract, while a shorter construct encompassing residues 15-43 is unable to do so (Figure 1B, lanes 2 and 3 respectively).

The minimal Aurora-A binding domain of human TPX2(1-43) is sufficient to stimulate the activity of the kinase *in vitro* (Figure 1C). Phosphorylation of histone H3, an Aurora-A substrate, is markedly increased by the addition of TPX2(1-43) (Figure 1C compare lane 1

with lane 3), but not by the shorter TPX2(15-43) (lane 4). Full-length TPX2 also increases the activity of the kinase, but appears less effective than the fragment. Full-length TPX2 may require additional factors such as microtubules for full activation. While microtubules can stimulate TPX2 activation of Aurora-A, no enhancement is detected for TPX2 1-43, which does not bind microtubules. Full-length TPX2 is itself a substrate for Aurora-A. The phosphorylation observed for GST-fused TPX2(1-43) (Figure 1C, lane 3) is however likely a non-specific artifact of the *in vitro* reaction because upon cleavage of the fusion protein phosphorylation signal is also detected on GST (lane 2). Furthermore, mass spectroscopy does not reveal Aurora-A phosphorylation sites in full-length TPX2.

The presence of TPX2(1-43) protects Aurora-A from deactivating dephosphorylation (Figure 1E). In the absence of TPX2, Aurora-A is completely dephosphorylated by phosphatase PP1 (lanes 1 and 2). In the presence of full-length TPX2, PP1 treatment dephosphorylates most sites of Aurora-A (lanes 3 and 4, upper panel) but prevents dephosphorylation of $Thr288^{AUR}$ (lane 4, lower panel, arrow). An even stronger protection effect is observed upon addition of TPX2(1-43) (lane 6). In the presence of TPX2 15-43, Aurora-A is fully dephosphorylated as in the absence of TPX2 altogether (lanes 8 and 2), consistent with the shorter fragment being unable to bind Aurora-A (Figure 1B). Thus, residues 1-43 of human TPX2 are necessary and sufficient for Aurora-A binding, activation and protection from dephosphorylation.

Overall structure of TPX2-bound Aurora-A

For crystallisation purposes, a minimal functional complex of Aurora-A and TPX2 was focused on. The N-terminus of Aurora-A is overall poorly conserved across species and is not required to bind TPX2. A fragment of Aurora-A lacking the N-terminus (residues 122-403, AuroraΔN) interacts with the active fragment of TPX2 (1-43) as efficiently as the full-length kinase (Figure 2A lanes 5 and 4). Both fragments are highly conserved (Figure 2D, 2E) and indeed *Xenopus* TPX2(1-39) can bind human AuroraΔN. AuroraΔN is phosphorylated when expressed in *E. coli*, as detected by a phospho-specific antibody (Figure 2B, lane 1). This appears to be due to Aurora-A autophosphorylation rather than to the activity of a bacterial kinase, since no phosphorylation can be detected upon expressing a mutant where an important catalytic residue, $Asp274^{AUR}$, has been mutated to Asn (Figure 2B, lane 2). The unphosphorylated mutant is catalytically inactive but retains TPX2-binding activity (Figure 2A, lane 6). AuroraΔN is activated by TPX2(1-43) (Figure 2C, lanes 2,3).

The complex between human phosphorylated AuroraΔN and TPX2(1-43) is active in histone H3 phosphorylation (Figure 2C, lane 7). The complex was crystallized in the presence of

Mg^{2+} ions and the ATP analogue ATPγS. The structure was determined by molecular replacement and refined it using 2.5 Å resolution data to a *R*free of 25.2% (see Table 1). The polypeptide model includes the catalytic core of the kinase (residues 123-387^{AUR}) and two segments of TPX2 (residues 7-21 ^{TPX} and 30-43^{TPX}). No ordered electron density is present for the eight intervening residues of TPX2 (22-29^{TPX}), which have therefore not been modelled.

The kinase catalytic core has an overall bilobate structure (Figure 3A,B). Briefly, the N-terminal lobe (residues 123-210) consists of a β-sheet and two α-helices, including the prominent helix αC whereas the C-terminal and larger lobe (residues 217-387) is mostly α-helical. The active site is situated at the interface between the lobes and includes the ATP-binding site, the catalytic base (Asp256^{AUR}) and the kinase activation segment (residues 274-299^{AUR}). In contrast to the structure of unphosphorylated Aurora-A, the activation segment is well ordered in the electron density and includes two phosphorylated threonine residues (Thr287^{AUR} and Thr288^{AUR}). Although the crystals were formed in the presence of ATP-γS, the electron density for the nucleotide reveals only the adenosine with two ordered phosphates and has been modelled as an ADP.

Specific recognition of TPX2 at two sites on Aurora-A

TPX2 binds Aurora-A with two separate stretches recognized at two distinct sites on the kinase. The upstream stretch (residues 7-21^{TPX}) binds at the N-terminal lobe of Aurora-A (Figure 3A,B). The downstream stretch (residues 30-43^{TPX}) binds in a α-helical conformation between the N- and C-terminal lobes (Figure 3A,B). The two Aurora-A-binding motifs of TPX2 appear to be connected by a flexible linker (disordered in the structure) that is variable in length and sequence across species (Figure 2D). Additionally, the two stretches are connected by an intramolecular hydrogen bond between Asp11^{TPX} and Trp34^{TPX}.

The upstream stretch of TPX2 has a mostly extended conformation, with a kink in the middle induced at a proline residue (Pro13^{TPX}) (for details see Figure 3C). The conserved segment ^{8}YSYDAPS^{14} (Figure 2D) is engaged in extensive main-chain and side-chain interactions with Aurora-A. In particular, Tyr8^{TPX}, Tyr10^{TPX} and Ala12^{TPX} tightly nestle into a hydrophobic groove between the β-sheet, helix αB and helix αC. An adjacent hydrophobic groove accommodates the side chains of TPX2 residues from Phe16^{TPX} to Phe19^{TPX}. The N-terminal residues of the Aurora-A catalytic core make key contributions to this interface, in particular with Arg126^{AUR} forming a cation-π interaction with Phe16^{TPX}.

The downstream helical stretch of TPX2 interacts with both helix αC and the activation segment of Aurora-A, bridging them (see Figure 3D for details). Most prominently, two conserved aromatic residues (Trp34^{TPX} and Phe35^{TPX}) interact with His187^{AUR} and His280^{AUR}, and Ala39^{TPX} additionally contacts the activation segment at Pro282^{AUR}. While the side of the TPX2 helix in contact with the kinase is lined by hydrophobic and conserved residues, the opposite side exposed to solvent comprises hydrophilic and variable residues. Residues 40-43^{TPX} at the end of the helix assume an extended conformation and are involved in contacts with a symmetry-related Aurora-A molecule within the crystal lattice.

TPX2 is phosphorylated in mitotic extracts and may well be regulated by phosphorylation. Even if TPX2 was phosphorylated in the first 43 residues, examination of the crystal structure suggests that the interaction of TPX2 with Aurora-A is unlikely to be regulated this way because all the conserved serine residues point towards solvent.

Phosphorylated Aurora-A is in an active conformation when bound to TPX2

Comparison with other kinase structures reveals that phosphorylated TPX2-bound Aurora-A closely matches the conformation of kinases in the active conformation. Using the program DALI (Holm and Sander, 1993), it was found particularly similar to cAMP-dependent protein kinase (PDB code 1YDS, 1.3 Å r.m.s.d., 257 structurally equivalent residues). Structural comparison shows that all the conserved residues at the active site are correctly oriented for catalysis (Figure 4A). These include the positively-charged residue aligning the phosphates for catalysis (Lys162^{AUR}, equivalent to Lys72^{cAPK}), the negatively-charged residue coordinating the magnesium ion bound to the nucleotide (Asp274^{AUR}, equivalent to Asp184^{cAPK}), and the catalytic base (Asp256^{AUR}, equivalent to Asp166^{cAPK}) whose role is to transfer the γ-phosphate of ATP to the hydroxyl group of a substrate serine or threonine residue.

The phosphorylated activation segment of TPX2-bound Aurora-A is in a conformation typical of active Ser/Thr kinases. It is virtually superposable to that of active cAPK (Figure 4A), with an r.m.s.d. of 0.8 Å between the Cα atoms of residues 274-299^{AUR} and 184-208^{cAPK}. In cAPK, the phosphorylated Thr197^{cAPK} interacts with Arg165^{cAPK} and with a basic surface patch (His87^{cAPK} and Lys189^{cAPK}), influencing the preceding catalytic residue (Asp166^{cAPK}). In Aurora-A, the phosphoryl moiety of Thr288^{AUR} is at the same structural position and interacts with the corresponding Arg255^{AUR} and with a similar, though not identical, basic patch (Arg180^{AUR} and Arg286^{AUR}), linking the catalytic residue (Asp256^{AUR}) to helix αC and to the activation segment. Mutation of Thr288^{AUR} to Asp generates a protein more active than

unphosphorylated wild-type Aurora-A, but much less active than the phosphorylated wild-type kinase. This mutation is thus a poor mimic of phosphorylation at Thr288^{AUR}, and although a Glu may potentially produce a stronger effect by more closely approximating the position of the phosphate, it would also be inadequate to balance the positive charges of the three surrounding arginines.

The phosphorylated activation segment of Aurora-A is in an inactive conformation in the absence of TPX2

To address the contribution of TPX2 to the conformation at the active site of TPX2-bound Aurora-A, the structure of phosphorylated AuroraΔN has been determined in the absence of TPX2. The model includes residues 127-389^{AUR} and has been refined at 2.75 Å resolution to an *R*free of 29.6% (Table 1). The overall structure of phosphorylated Aurora-A is similar for the TPX2-bound and unbound forms. The two lobes of the kinase have the same relative orientation and helix αC does not change conformation upon binding the regulator (Figure 4A). Overall, more than 95% of the amino-acid residues superpose with an overall r.m.s.d. of 0.9 Å. However, the two structures differ significantly in the activation segment.

The phosphorylated activation segments of Aurora-A in the TPX2-bound state (Figure 4A) and unbound state (Figure 4A) diverge between residues His280^{AUR} and Leu293^{AUR} (rmsd of 5.4 Å). In the absence of TPX2, the phosphorylated Thr288^{AUR} is exposed to solvent rather than pointing towards Arg255^{AUR} as observed when TPX2 is bound (Figure 4A). The region of the activation segment around the phosphorylated Thr288^{AUR} (residues 286-291^{AUR}) is relatively disordered, with average B-factors of 85 Å^2 as compared with 53 Å^2 for the rest of the molecule. However, the tracing of the polypeptide chain is unambiguous and this fragment of the activation segment is overall less closely packed to the C-terminal lobe of the kinase. The segment becomes well ordered again at Thr292^{AUR} and Leu293^{AUR}. This part of the activation segment is in a different conformation with respect to the TPX2-bound form (Figure 4A), with Thr292^{AUR} being unable to hydrogen bond and thus influence the catalytic Asp256^{AUR} (Figure 4A). This conformation seems to be stabilized by the movement of Leu293^{AUR}, which inserts its side chain into a small apolar pocket. The presence of a Leu at this position is uncommon in other kinases, which typically have a Pro residue instead (cAPK, for example, Figures 2E). A further movement of residues 298-306 accommodates changes in the adjacent activation segment, and leads to the formation of a Glu302-His366 interaction. This interaction may be affected by the negative charge introduced in the S349D mutant of *Xenopus* Aurora-A explaining why this mutant is catalytically inactive.

Structural basis for the activation of Aurora-A by TPX2

Comparison of phosphorylated Aurora-A in the unbound and TPX2-bound forms reveals the molecular basis for the enhancement of kinase activity. In the absence of TPX2, the crucial phosphothreonine does not bind to helix αC and the activation segment overlaps with the substrate-binding site rather than providing a substrate-binding platform. The phosphorylated $Thr288^{AUR}$ has no direct connection with TPX2, the phosphate moiety being 14 Å from the nearest TPX2 atom. Nonetheless, TPX2 induces a 10 Å movement of the phosphoryl moiety required to achieve the active conformation (Figure 4B).

The helical stretch of TPX2 contacts the activation segment at $His280^{AUR}$ and $Pro282^{AUR}$, which appear to be the pivot points of the conformational change (Figures 4B, 4C). In essence, a rotation about $His280^{AUR}$ swings $Pro282^{AUR}$ and $Ser283^{AUR}$ towards the TPX2 helix, pulling downstream residues of the activation segment to pack more closely with the kinase core (Figure 4B). In this lever-arm-like mechanism, a small change at the pivot points ($His280^{AUR}$, $Pro282^{AUR}$) produces a large movement in the arm (P-$Thr288^{AUR}$ Figure 4C). While in the unbound form the activation segment is rather mobile and has probably sufficient conformational freedom to adopt an active conformation in the presence of substrate (basal kinase activity, Figure 1C, lane 1), in the TPX2-bound form, the active conformation is ready for substrate binding and catalysis (increased kinase activity, Figure 1C, lanes 2 and 3). The C-terminal residues ($40\text{-}43^{TPX}$) protruding from a neighbouring TPX2 molecule in the crystals bind to the activation segment, albeit in the opposite main chain direction to a real substrate. Substrate binding alone does not fully activate Aurora-A in solution (Figure 1C), and it is therefore very unlikely that this substrate-like contact is responsible for the active conformation in the crystal structure. Substrate binding, however, might assist in inducing an active conformation, especially in the absence of TPX2.

In addition to enhancing the activity of Aurora-A, TPX2 also protects the kinase from dephosphorylation by phosphatases. The site for PP1 binding on Aurora-A is mapped to the C-terminus, a region that is distant from the TPX2 binding site and that is structurally unaffected upon binding of the regulator. Thus TPX2 is unlikely to protect Aurora-A from dephosphorylation by preventing phosphatase binding. Indeed, even in the presence of TPX2, the phosphatase is capable of removing the phosphates from most side chains with the exception of $Thr288^{AUR}$ (Figure 1E). TPX2 prevents $Thr288^{AUR}$ dephosphorylation by moving the phosphate moiety from a solvent-exposed position to a buried position, which is inaccessible to an incoming phosphatase. The other phosphorylated threonine in the kinase catalytic core, $Thr287^{AUR}$, is conspicuously exposed to solvent and may serve as a decoy to further mask $Thr288^{AUR}$ (Figure 3B).

Table 1. Summary of crystallographic analysis

		Phospho-Aurora-A + TPX2	Phospho-Aurora-A
Crystals			
Spacegroup		$P2_12_12_1$	$P6_122$
Lattice constants	*a* (Å)	59.63	81.18
	b (Å)	81.72	81.18
	c (Å)	83.05	169.62
Data collection			
X-ray source		SLS XO6SA	ESRF ID14EH1
Resolution range (Å)		40-2.5	70-2.75
(Highest resolution shell)		(2.64-2.5)	(2.9-2.75)
Unique reflections		14609	9235
Completeness(%)		100 (100)	100 (100)
Multiplicity		5.6 (5.7)	10.1 (10.6)
Rmerge (%)		9.9 (24.8)	11.9 (34.6)
I/σ(I)		5.1 (1.1)	3.8 (2.1)
Refinement			
Resolution range (Å)		40-2.5	20-2.75
Number of residues		294	263
Number of waters		144	9
*R*factor (%)		19.4	25.7
*R*free[a] (%)		25.2	29.6
Ramachandran plot			
Most favoured (%)		91.5	82.4
Allowed (%)		8.1	16.3
Generously allowed (%)		0.0	0.9
Forbidden (%)		0.4[b]	0.4[b]

[a] Free *R*factor was computed using 5% of the data assigned randomly (Brunger, 1992).

[b] $Ser226^{AUR}$ resides in a loop and the conformation is supported by excellent electron density.

Table A

ATOM	1	CB	GLN	A	127	267.519	-61.189	87.734	1.00	66.58	A
C										
ATOM	2	CG	GLN	A	127	266.971	-61.391	86.330	1.00	76.29	A
C										
ATOM	3	CD	GLN	A	127	266.372	-60.121	85.741	1.00	79.34	A
C										
ATOM	4	OE1	GLN	A	127	265.589	-60.183	84.781	1.00	82.34	A
O										
ATOM	5	NE2	GLN	A	127	266.735	-58.962	86.307	1.00	82.40	A
N										
ATOM	6	C	GLN	A	127	269.192	-59.883	89.051	1.00	63.35	A
C										
ATOM	7	O	GLN	A	127	269.877	-58.853	89.024	1.00	70.04	A
O										
ATOM	8	N	GLN	A	127	269.910	-61.949	87.808	1.00	58.04	A
N										
ATOM	9	CA	GLN	A	127	269.002	-60.755	87.810	1.00	67.74	A
C										
ATOM	10	N	TRP	A	128	268.566	-60.307	90.137	1.00	61.21	A
N										
ATOM	11	CA	TRP	A	128	268.621	-59.552	91.366	1.00	53.96	A
C										
ATOM	12	CB	TRP	A	128	267.315	-59.733	92.133	1.00	50.38	A
C										
ATOM	13	CG	TRP	A	128	266.140	-59.256	91.369	1.00	49.11	A
C										
ATOM	14	CD2	TRP	A	128	265.908	-57.928	90.897	1.00	50.34	A
C										
ATOM	15	CE2	TRP	A	128	264.697	-57.962	90.150	1.00	53.33	A
C										
ATOM	16	CE3	TRP	A	128	266.611	-56.713	91.017	1.00	53.44	A
C										
ATOM	17	CD1	TRP	A	128	265.096	-60.014	90.921	1.00	47.17	A
C										
ATOM	18	NE1	TRP	A	128	264.228	-59.249	90.191	1.00	49.20	A
N										
ATOM	19	CZ2	TRP	A	128	264.160	-56.816	89.514	1.00	56.77	A
C										
ATOM	20	CZ3	TRP	A	128	266.094	-55.571	90.392	1.00	60.23	A
C										
ATOM	21	CH2	TRP	A	128	264.869	-55.633	89.639	1.00	61.57	A
C										
ATOM	22	C	TRP	A	128	269.787	-59.909	92.262	1.00	54.43	A
C										
ATOM	23	O	TRP	A	128	270.317	-61.026	92.231	1.00	54.76	A
O										
ATOM	24	N	ALA	A	129	270.184	-58.955	93.085	1.00	55.48	A
N										
ATOM	25	CA	ALA	A	129	271.283	-59.206	94.006	1.00	60.01	A
C										
ATOM	26	CB	ALA	A	129	272.608	-58.800	93.341	1.00	66.60	A
C										
ATOM	27	C	ALA	A	129	271.010	-58.371	95.258	1.00	56.86	A
C										
ATOM	28	O	ALA	A	129	270.365	-57.326	95.173	1.00	59.08	A
O										
ATOM	29	N	LEU	A	130	271.517	-58.821	96.401	1.00	51.68	A
N										
ATOM	30	CA	LEU	A	130	271.314	-58.126	97.665	1.00	53.06	A
C										

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ATOM     31  CB  LEU A 130     272.108 -58.770  98.787  1.00 43.18      A
C
ATOM     32  CG  LEU A 130     272.080 -58.110 100.164  1.00 36.68      A
C
ATOM     33  CD1 LEU A 130     270.621 -57.934 100.570  1.00 47.13      A
C
ATOM     34  CD2 LEU A 130     272.839 -58.975 101.186  1.00 38.64      A
C
ATOM     35  C   LEU A 130     271.750 -56.702  97.591  1.00 55.17      A
C
ATOM     36  O   LEU A 130     271.223 -55.834  98.305  1.00 61.19      A
O
ATOM     37  N   GLU A 131     272.686 -56.469  96.690  1.00 58.94      A
N
ATOM     38  CA  GLU A 131     273.276 -55.172  96.539  1.00 57.04      A
C
ATOM     39  CB  GLU A 131     274.689 -55.400  96.030  1.00 63.45      A
C
ATOM     40  CG  GLU A 131     275.441 -56.450  96.938  1.00 73.38      A
C
ATOM     41  CD  GLU A 131     275.249 -57.909  96.486  1.00 79.54      A
C
ATOM     42  OE1 GLU A 131     274.529 -58.142  95.477  1.00 80.97      A
O
ATOM     43  OE2 GLU A 131     275.838 -58.820  97.135  1.00 88.53      A
O
ATOM     44  C   GLU A 131     272.458 -54.235  95.682  1.00 55.07      A
C
ATOM     45  O   GLU A 131     272.851 -53.119  95.439  1.00 51.83      A
O
ATOM     46  N   ASP A 132     271.280 -54.704  95.299  1.00 53.60      A
N
ATOM     47  CA  ASP A 132     270.298 -53.994  94.487  1.00 58.59      A
C
ATOM     48  CB  ASP A 132     269.514 -54.987  93.656  1.00 69.09      A
C
ATOM     49  CG  ASP A 132     270.030 -55.141  92.284  1.00 68.36      A
C
ATOM     50  OD1 ASP A 132     269.776 -54.250  91.447  1.00 73.44      A
O
ATOM     51  OD2 ASP A 132     270.704 -56.159  92.048  1.00 76.16      A
O
ATOM     52  C   ASP A 132     269.267 -53.412  95.449  1.00 59.74      A
C
ATOM     53  O   ASP A 132     268.472 -52.547  95.093  1.00 56.43      A
O
ATOM     54  N   PHE A 133     269.239 -53.925  96.666  1.00 62.15      A
N
ATOM     55  CA  PHE A 133     268.239 -53.448  97.598  1.00 62.91      A
C
ATOM     56  CB  PHE A 133     267.324 -54.622  97.974  1.00 59.55      A
C
ATOM     57  CG  PHE A 133     266.737 -55.337  96.775  1.00 61.26      A
C
ATOM     58  CD1 PHE A 133     267.467 -56.312  96.095  1.00 60.00      A
C
ATOM     59  CD2 PHE A 133     265.442 -55.059  96.346  1.00 60.03      A
C
ATOM     60  CE1 PHE A 133     266.910 -56.996  94.991  1.00 65.06      A
C
ATOM     61  CE2 PHE A 133     264.883 -55.719  95.264  1.00 60.82      A
C
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ATOM     62  CZ  PHE A 133     265.607 -56.697  94.585  1.00 61.32      A
C
ATOM     63  C   PHE A 133     268.740 -52.733  98.847  1.00 61.07      A
C
ATOM     64  O   PHE A 133     269.866 -52.972  99.318  1.00 66.24      A
O
ATOM     65  N   GLU A 134     267.878 -51.829  99.340  1.00 59.55      A
N
ATOM     66  CA  GLU A 134     268.062 -51.035 100.573  1.00 58.90      A
C
ATOM     67  CB  GLU A 134     267.589 -49.593 100.353  1.00 54.77      A
C
ATOM     68  CG  GLU A 134     268.478 -48.772  99.488  1.00 63.45      A
C
ATOM     69  CD  GLU A 134     268.205 -47.282  99.556  1.00 61.84      A
C
ATOM     70  OE1 GLU A 134     268.808 -46.576 100.384  1.00 75.06      A
O
ATOM     71  OE2 GLU A 134     267.388 -46.803  98.768  1.00 73.27      A
O
ATOM     72  C   GLU A 134     267.139 -51.698 101.627  1.00 53.85      A
C
ATOM     73  O   GLU A 134     265.909 -51.607 101.526  1.00 60.03      A
O
ATOM     74  N   ILE A 135     267.713 -52.362 102.621  1.00 52.32      A
N
ATOM     75  CA  ILE A 135     266.917 -53.042 103.625  1.00 50.89      A
C
ATOM     76  CB  ILE A 135     267.750 -54.131 104.343  1.00 48.23      A
C
ATOM     77  CG2 ILE A 135     266.828 -55.078 105.127  1.00 51.35      A
C
ATOM     78  CG1 ILE A 135     268.552 -54.940 103.317  1.00 48.00      A
C
ATOM     79  CD1 ILE A 135     267.731 -55.720 102.398  1.00 35.46      A
C
ATOM     80  C   ILE A 135     266.298 -52.129 104.674  1.00 50.54      A
C
ATOM     81  O   ILE A 135     266.973 -51.281 105.250  1.00 50.32      A
O
ATOM     82  N   GLY A 136     265.004 -52.334 104.924  1.00 49.85      A
N
ATOM     83  CA  GLY A 136     264.286 -51.534 105.903  1.00 44.78      A
C
ATOM     84  C   GLY A 136     264.165 -52.255 107.228  1.00 44.85      A
C
ATOM     85  O   GLY A 136     265.040 -53.071 107.574  1.00 45.10      A
O
ATOM     86  N   ARG A 137     263.071 -51.996 107.940  1.00 40.54      A
N
ATOM     87  CA  ARG A 137     262.891 -52.598 109.248  1.00 47.22      A
C
ATOM     88  CB  ARG A 137     261.911 -51.766 110.065  1.00 46.15      A
C
ATOM     89  CG  ARG A 137     260.481 -51.887 109.585  1.00 46.77      A
C
ATOM     90  CD  ARG A 137     259.521 -51.284 110.589  1.00 47.76      A
C
ATOM     91  NE  ARG A 137     258.174 -51.283 110.058  1.00 44.18      A
N
ATOM     92  CZ  ARG A 137     257.364 -52.330 110.097  1.00 49.13      A
C
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ATOM	93	NH1	ARG	A	137	257.779	-53.468	110.655	1.00	50.41	A
N											
ATOM	94	NH2	ARG	A	137	256.144	-52.230	109.579	1.00	42.98	A
N											
ATOM	95	C	ARG	A	137	262.358	-54.014	109.150	1.00	48.40	A
C											
ATOM	96	O	ARG	A	137	261.734	-54.370	108.150	1.00	52.53	A
O											
ATOM	97	N	PRO	A	138	262.589	-54.840	110.190	1.00	48.54	A
N											
ATOM	98	CD	PRO	A	138	263.443	-54.581	111.363	1.00	46.06	A
C											
ATOM	99	CA	PRO	A	138	262.108	-56.226	110.213	1.00	46.02	A
C											
ATOM	100	CB	PRO	A	138	262.685	-56.765	111.524	1.00	49.55	A
C											
ATOM	101	CG	PRO	A	138	263.905	-55.955	111.710	1.00	42.97	A
C											
ATOM	102	C	PRO	A	138	260.561	-56.262	110.207	1.00	49.85	A
C											
ATOM	103	O	PRO	A	138	259.920	-55.810	111.142	1.00	50.42	A
O											
ATOM	104	N	LEU	A	139	259.980	-56.799	109.138	1.00	45.75	A
N											
ATOM	105	CA	LEU	A	139	258.545	-56.896	109.005	1.00	39.58	A
C											
ATOM	106	CB	LEU	A	139	258.181	-57.130	107.558	1.00	37.24	A
C											
ATOM	107	CG	LEU	A	139	258.109	-55.885	106.664	1.00	42.68	A
C											
ATOM	108	CD1	LEU	A	139	257.816	-56.315	105.170	1.00	32.13	A
C											
ATOM	109	CD2	LEU	A	139	256.990	-54.961	107.170	1.00	43.77	A
C											
ATOM	110	C	LEU	A	139	257.968	-58.002	109.880	1.00	40.81	A
C											
ATOM	111	O	LEU	A	139	256.907	-57.861	110.480	1.00	45.92	A
O											
ATOM	112	N	GLY	A	140	258.675	-59.111	109.970	1.00	45.15	A
N											
ATOM	113	CA	GLY	A	140	258.198	-60.218	110.789	1.00	48.82	A
C											
ATOM	114	C	GLY	A	140	259.222	-61.317	111.040	1.00	48.37	A
C											
ATOM	115	O	GLY	A	140	260.326	-61.310	110.492	1.00	53.08	A
O											
ATOM	116	N	LYS	A	141	258.842	-62.283	111.856	1.00	52.66	A
N											
ATOM	117	CA	LYS	A	141	259.740	-63.376	112.192	1.00	56.79	A
C											
ATOM	118	CB	LYS	A	141	259.961	-63.404	113.707	1.00	61.89	A
C											
ATOM	119	CG	LYS	A	141	260.862	-64.513	114.210	1.00	68.25	A
C											
ATOM	120	CD	LYS	A	141	260.894	-64.538	115.750	1.00	78.79	A
C											
ATOM	121	CE	LYS	A	141	261.863	-65.624	116.242	1.00	83.42	A
C											
ATOM	122	NZ	LYS	A	141	261.987	-65.651	117.745	1.00	90.84	A
N											
ATOM	123	C	LYS	A	141	259.219	-64.728	111.704	1.00	57.82	A
C											

ATOM	124	O	LYS	A	141	258.150	-65.199	112.084	1.00	57.17	A
O											
ATOM	125	N	GLY	A	142	259.990	-65.342	110.823	1.00	63.79	A
N											
ATOM	126	CA	GLY	A	142	259.627	-66.648	110.315	1.00	67.77	A
C											
ATOM	127	C	GLY	A	142	260.381	-67.717	111.087	1.00	68.12	A
C											
ATOM	128	O	GLY	A	142	260.756	-67.533	112.255	1.00	76.19	A
O											
ATOM	129	N	LYS	A	143	260.638	-68.829	110.410	1.00	66.29	A
N											
ATOM	130	CA	LYS	A	143	261.359	-69.941	111.016	1.00	62.91	A
C											
ATOM	131	CB	LYS	A	143	260.576	-71.221	110.783	1.00	56.50	A
C											
ATOM	132	CG	LYS	A	143	260.990	-72.331	111.694	1.00	59.59	A
C											
ATOM	133	CD	LYS	A	143	259.804	-73.170	112.130	1.00	65.95	A
C											
ATOM	134	CE	LYS	A	143	260.182	-74.141	113.303	1.00	69.37	A
C											
ATOM	135	NZ	LYS	A	143	259.069	-75.109	113.596	1.00	70.95	A
N											
ATOM	136	C	LYS	A	143	262.773	-70.081	110.500	1.00	62.52	A
C											
ATOM	137	O	LYS	A	143	263.725	-70.302	111.243	1.00	61.60	A
O											
ATOM	138	N	PHE	A	144	262.909	-69.898	109.200	1.00	68.60	A
N											
ATOM	139	CA	PHE	A	144	264.215	-70.021	108.556	1.00	74.62	A
C											
ATOM	140	CB	PHE	A	144	264.109	-70.886	107.296	1.00	69.32	A
C											
ATOM	141	CG	PHE	A	144	263.583	-72.278	107.565	1.00	69.58	A
C											
ATOM	142	CD1	PHE	A	144	262.211	-72.526	107.690	1.00	66.23	A
C											
ATOM	143	CD2	PHE	A	144	264.460	-73.335	107.731	1.00	63.51	A
C											
ATOM	144	CE1	PHE	A	144	261.738	-73.816	107.978	1.00	73.24	A
C											
ATOM	145	CE2	PHE	A	144	263.985	-74.608	108.014	1.00	69.83	A
C											
ATOM	146	CZ	PHE	A	144	262.629	-74.850	108.138	1.00	66.31	A
C											
ATOM	147	C	PHE	A	144	264.768	-68.665	108.234	1.00	74.80	A
C											
ATOM	148	O	PHE	A	144	265.636	-68.496	107.395	1.00	82.71	A
O											
ATOM	149	N	GLY	A	145	264.248	-67.691	108.955	1.00	83.57	A
N											
ATOM	150	CA	GLY	A	145	264.676	-66.320	108.782	1.00	77.10	A
C											
ATOM	151	C	GLY	A	145	263.544	-65.296	108.827	1.00	75.14	A
C											
ATOM	152	O	GLY	A	145	262.338	-65.557	108.521	1.00	74.64	A
O											
ATOM	153	N	ASN	A	146	263.966	-64.097	109.195	1.00	67.46	A
N											
ATOM	154	CA	ASN	A	146	263.050	-62.976	109.318	1.00	65.84	A
C											

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ATOM    155  CB  ASN A 146     263.674 -61.895 110.208  1.00 68.52      A
C
ATOM    156  CG  ASN A 146     263.873 -62.369 111.664  1.00 74.23      A
C
ATOM    157  OD1 ASN A 146     264.045 -63.577 111.946  1.00 76.10      A
O
ATOM    158  ND2 ASN A 146     263.871 -61.415 112.588  1.00 74.93      A
N
ATOM    159  C   ASN A 146     262.727 -62.402 107.955  1.00 60.10      A
C
ATOM    160  O   ASN A 146     263.442 -62.661 106.979  1.00 60.40      A
O
ATOM    161  N   VAL A 147     261.651 -61.614 107.909  1.00 49.34      A
N
ATOM    162  CA  VAL A 147     261.208 -60.938 106.697  1.00 34.29      A
C
ATOM    163  CB  VAL A 147     259.691 -61.195 106.433  1.00 35.55      A
C
ATOM    164  CG1 VAL A 147     259.202 -60.303 105.293  1.00 22.76      A
C
ATOM    165  CG2 VAL A 147     259.444 -62.657 106.040  1.00 25.36      A
C
ATOM    166  C   VAL A 147     261.432 -59.427 106.905  1.00 36.01      A
C
ATOM    167  O   VAL A 147     261.071 -58.888 107.912  1.00 33.80      A
O
ATOM    168  N   TYR A 148     262.006 -58.743 105.931  1.00 38.73      A
N
ATOM    169  CA  TYR A 148     262.298 -57.313 106.040  1.00 38.16      A
C
ATOM    170  CB  TYR A 148     263.815 -57.053 105.947  1.00 44.86      A
C
ATOM    171  CG  TYR A 148     264.625 -57.783 106.981  1.00 51.34      A
C
ATOM    172  CD1 TYR A 148     264.946 -59.110 106.823  1.00 49.12      A
C
ATOM    173  CE1 TYR A 148     265.660 -59.799 107.804  1.00 57.49      A
C
ATOM    174  CD2 TYR A 148     265.035 -57.152 108.146  1.00 56.42      A
C
ATOM    175  CE2 TYR A 148     265.743 -57.839 109.136  1.00 62.05      A
C
ATOM    176  CZ  TYR A 148     266.051 -59.159 108.958  1.00 59.22      A
C
ATOM    177  OH  TYR A 148     266.740 -59.818 109.951  1.00 62.90      A
O
ATOM    178  C   TYR A 148     261.647 -56.485 104.972  1.00 40.31      A
C
ATOM    179  O   TYR A 148     261.240 -56.989 103.910  1.00 39.68      A
O
ATOM    180  N   LEU A 149     261.564 -55.187 105.254  1.00 37.70      A
N
ATOM    181  CA  LEU A 149     260.992 -54.236 104.287  1.00 36.17      A
C
ATOM    182  CB  LEU A 149     260.495 -52.976 105.019  1.00 38.73      A
C
ATOM    183  CG  LEU A 149     259.781 -51.920 104.186  1.00 39.39      A
C
ATOM    184  CD1 LEU A 149     258.437 -52.465 103.793  1.00 46.05      A
C
ATOM    185  CD2 LEU A 149     259.655 -50.660 104.957  1.00 40.68      A
C
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ATOM	186	C	LEU	A	149	262.212	-53.920	103.405	1.00	35.83	A
C											
ATOM	187	O	LEU	A	149	263.340	-54.217	103.822	1.00	37.60	A
O											
ATOM	188	N	ALA	A	150	262.029	-53.321	102.228	1.00	37.02	A
N											
ATOM	189	CA	ALA	A	150	263.171	-53.041	101.363	1.00	35.35	A
C											
ATOM	190	CB	ALA	A	150	263.889	-54.345	100.965	1.00	48.80	A
C											
ATOM	191	C	ALA	A	150	262.746	-52.334	100.123	1.00	44.17	A
C											
ATOM	192	O	ALA	A	150	261.665	-52.604	99.566	1.00	41.00	A
O											
ATOM	193	N	ARG	A	151	263.619	-51.441	99.666	1.00	47.00	A
N											
ATOM	194	CA	ARG	A	151	263.319	-50.674	98.468	1.00	50.37	A
C											
ATOM	195	CB	ARG	A	151	263.377	-49.171	98.793	1.00	53.91	A
C											
ATOM	196	CG	ARG	A	151	262.912	-48.272	97.649	1.00	53.96	A
C											
ATOM	197	CD	ARG	A	151	262.884	-46.817	98.014	1.00	57.39	A
C											
ATOM	198	NE	ARG	A	151	264.145	-46.372	98.607	1.00	58.37	A
N											
ATOM	199	CZ	ARG	A	151	264.561	-45.110	98.572	1.00	58.07	A
C											
ATOM	200	NH1	ARG	A	151	263.814	-44.175	97.969	1.00	56.20	A
N											
ATOM	201	NH2	ARG	A	151	265.718	-44.793	99.131	1.00	55.48	A
N											
ATOM	202	C	ARG	A	151	264.311	-51.021	97.348	1.00	55.38	A
C											
ATOM	203	O	ARG	A	151	265.503	-51.247	97.625	1.00	60.78	A
O											
ATOM	204	N	GLU	A	152	263.826	-51.059	96.105	1.00	54.28	A
N											
ATOM	205	CA	GLU	A	152	264.664	-51.366	94.972	1.00	54.46	A
C											
ATOM	206	CB	GLU	A	152	263.811	-51.817	93.823	1.00	60.23	A
C											
ATOM	207	CG	GLU	A	152	264.520	-52.780	92.888	1.00	67.69	A
C											
ATOM	208	CD	GLU	A	152	265.617	-52.120	92.087	1.00	75.21	A
C											
ATOM	209	OE1	GLU	A	152	266.773	-52.020	92.593	1.00	78.70	A
O											
ATOM	210	OE2	GLU	A	152	265.305	-51.689	90.951	1.00	76.28	A
O											
ATOM	211	C	GLU	A	152	265.436	-50.117	94.598	1.00	54.18	A
C											
ATOM	212	O	GLU	A	152	264.868	-49.045	94.388	1.00	55.50	A
O											
ATOM	213	N	LYS	A	153	266.746	-50.275	94.489	1.00	55.96	A
N											
ATOM	214	CA	LYS	A	153	267.583	-49.115	94.231	1.00	57.21	A
C											
ATOM	215	CB	LYS	A	153	269.059	-49.471	94.257	1.00	56.21	A
C											
ATOM	216	CG	LYS	A	153	269.661	-49.042	95.586	1.00	49.03	A
C											

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ATOM    217  CD  LYS A 153     270.821 -49.929  95.975  1.00 56.59      A
C
ATOM    218  CE  LYS A 153     271.022 -49.981  97.450  1.00 62.23      A
C
ATOM    219  NZ  LYS A 153     272.289 -50.704  97.804  1.00 63.82      A
N
ATOM    220  C   LYS A 153     267.300 -48.233  93.056  1.00 60.69      A
C
ATOM    221  O   LYS A 153     267.418 -47.029  93.188  1.00 68.16      A
O
ATOM    222  N   GLN A 154     266.890 -48.704  91.909  1.00 60.83      A
N
ATOM    223  CA  GLN A 154     266.722 -47.630  90.954  1.00 60.63      A
C
ATOM    224  CB  GLN A 154     267.313 -48.015  89.612  1.00 65.34      A
C
ATOM    225  CG  GLN A 154     268.585 -48.908  89.762  1.00 73.31      A
C
ATOM    226  CD  GLN A 154     268.842 -49.643  88.514  1.00 76.62      A
C
ATOM    227  OE1 GLN A 154     268.751 -49.059  87.368  1.00 77.22      A
O
ATOM    228  NE2 GLN A 154     269.150 -50.963  88.658  1.00 79.75      A
N
ATOM    229  C   GLN A 154     265.288 -47.279  90.868  1.00 58.41      A
C
ATOM    230  O   GLN A 154     264.929 -46.135  90.760  1.00 66.80      A
O
ATOM    231  N   SER A 155     264.465 -48.297  91.026  1.00 63.11      A
N
ATOM    232  CA  SER A 155     263.012 -48.182  90.986  1.00 57.08      A
C
ATOM    233  CB  SER A 155     262.438 -49.593  90.891  1.00 57.59      A
C
ATOM    234  OG  SER A 155     261.096 -49.532  90.511  1.00 71.09      A
O
ATOM    235  C   SER A 155     262.393 -47.454  92.192  1.00 54.17      A
C
ATOM    236  O   SER A 155     261.494 -46.653  92.054  1.00 41.48      A
O
ATOM    237  N   LYS A 156     262.919 -47.739  93.368  1.00 54.36      A
N
ATOM    238  CA  LYS A 156     262.415 -47.187  94.614  1.00 65.54      A
C
ATOM    239  CB  LYS A 156     262.133 -45.687  94.476  1.00 68.88      A
C
ATOM    240  CG  LYS A 156     263.375 -44.809  94.527  1.00 68.98      A
C
ATOM    241  CD  LYS A 156     263.018 -43.342  94.698  1.00 65.67      A
C
ATOM    242  CE  LYS A 156     262.170 -42.850  93.529  1.00 62.20      A
C
ATOM    243  NZ  LYS A 156     261.774 -41.416  93.679  1.00 56.13      A
N
ATOM    244  C   LYS A 156     261.138 -47.958  95.009  1.00 64.77      A
C
ATOM    245  O   LYS A 156     260.317 -47.485  95.803  1.00 68.30      A
O
ATOM    246  N   PHE A 157     261.012 -49.159  94.446  1.00 62.48      A
N
ATOM    247  CA  PHE A 157     259.891 -50.051  94.679  1.00 52.64      A
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ATOM    248  CB  PHE A 157     259.878 -51.110  93.580  1.00 54.51      A
C
ATOM    249  CG  PHE A 157     258.621 -51.933  93.525  1.00 52.32      A
C
ATOM    250  CD1 PHE A 157     257.665 -51.694  92.549  1.00 54.81      A
C
ATOM    251  CD2 PHE A 157     258.395 -52.950  94.448  1.00 55.89      A
C
ATOM    252  CE1 PHE A 157     256.499 -52.451  92.487  1.00 53.63      A
C
ATOM    253  CE2 PHE A 157     257.232 -53.719  94.401  1.00 54.27      A
C
ATOM    254  CZ  PHE A 157     256.286 -53.467  93.419  1.00 58.00      A
C
ATOM    255  C   PHE A 157     260.015 -50.719  96.056  1.00 51.79      A
C
ATOM    256  O   PHE A 157     261.020 -51.370  96.340  1.00 47.35      A
O
ATOM    257  N   ILE A 158     258.996 -50.539  96.900  1.00 50.33      A
N
ATOM    258  CA  ILE A 158     258.997 -51.137  98.212  1.00 48.14      A
C
ATOM    259  CB  ILE A 158     258.329 -50.196  99.284  1.00 48.26      A
C
ATOM    260  CG2 ILE A 158     257.863 -50.988 100.478  1.00 42.57      A
C
ATOM    261  CG1 ILE A 158     259.382 -49.205  99.795  1.00 48.74      A
C
ATOM    262  CD1 ILE A 158     258.914 -48.326 100.849  1.00 60.25      A
C
ATOM    263  C   ILE A 158     258.354 -52.530  98.176  1.00 52.33      A
C
ATOM    264  O   ILE A 158     257.269 -52.732  97.635  1.00 50.55      A
O
ATOM    265  N   LEU A 159     259.034 -53.472  98.823  1.00 52.37      A
N
ATOM    266  CA  LEU A 159     258.631 -54.858  98.835  1.00 48.01      A
C
ATOM    267  CB  LEU A 159     259.322 -55.530  97.663  1.00 49.17      A
C
ATOM    268  CG  LEU A 159     260.759 -55.019  97.480  1.00 47.74      A
C
ATOM    269  CD1 LEU A 159     261.690 -55.880  98.307  1.00 46.92      A
C
ATOM    270  CD2 LEU A 159     261.150 -55.055  96.008  1.00 47.94      A
C
ATOM    271  C   LEU A 159     259.089 -55.468 100.111  1.00 44.03      A
C
ATOM    272  O   LEU A 159     259.595 -54.777 100.931  1.00 48.23      A
O
ATOM    273  N   ALA A 160     258.889 -56.765 100.280  1.00 43.85      A
N
ATOM    274  CA  ALA A 160     259.347 -57.465 101.474  1.00 37.28      A
C
ATOM    275  CB  ALA A 160     258.187 -58.117 102.184  1.00 41.03      A
C
ATOM    276  C   ALA A 160     260.346 -58.531 101.030  1.00 43.40      A
C
ATOM    277  O   ALA A 160     260.084 -59.301 100.096  1.00 40.92      A
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ATOM    278  N   LEU A 161     261.494 -58.566 101.693  1.00 46.08      A
N
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ATOM	279	CA	LEU	A	161	262.564	-59.520	101.378	1.00	44.64	A
C											
ATOM	280	CB	LEU	A	161	263.916	-58.794	101.334	1.00	47.23	A
C											
ATOM	281	CG	LEU	A	161	264.865	-59.050	100.188	1.00	47.49	A
C											
ATOM	282	CD1	LEU	A	161	264.153	-58.846	98.870	1.00	42.04	A
C											
ATOM	283	CD2	LEU	A	161	266.031	-58.125	100.309	1.00	46.85	A
C											
ATOM	284	C	LEU	A	161	262.607	-60.592	102.441	1.00	45.60	A
C											
ATOM	285	O	LEU	A	161	263.013	-60.338	103.570	1.00	56.35	A
O											
ATOM	286	N	LYS	A	162	262.194	-61.801	102.078	1.00	46.81	A
N											
ATOM	287	CA	LYS	A	162	262.178	-62.940	103.009	1.00	41.78	A
C											
ATOM	288	CB	LYS	A	162	261.104	-63.922	102.585	1.00	37.22	A
C											
ATOM	289	CG	LYS	A	162	260.826	-65.007	103.588	1.00	34.96	A
C											
ATOM	290	CD	LYS	A	162	259.600	-65.804	103.219	1.00	30.75	A
C											
ATOM	291	CE	LYS	A	162	259.522	-67.056	104.081	1.00	32.45	A
C											
ATOM	292	NZ	LYS	A	162	258.194	-67.801	103.796	1.00	32.97	A
N											
ATOM	293	C	LYS	A	162	263.521	-63.634	103.018	1.00	43.17	A
C											
ATOM	294	O	LYS	A	162	263.869	-64.350	102.087	1.00	50.65	A
O											
ATOM	295	N	VAL	A	163	264.299	-63.369	104.049	1.00	47.41	A
N											
ATOM	296	CA	VAL	A	163	265.625	-63.965	104.187	1.00	50.56	A
C											
ATOM	297	CB	VAL	A	163	266.539	-63.091	105.120	1.00	49.49	A
C											
ATOM	298	CG1	VAL	A	163	267.951	-63.664	105.180	1.00	43.15	A
C											
ATOM	299	CG2	VAL	A	163	266.555	-61.660	104.586	1.00	46.95	A
C											
ATOM	300	C	VAL	A	163	265.570	-65.371	104.756	1.00	48.41	A
C											
ATOM	301	O	VAL	A	163	264.994	-65.586	105.798	1.00	53.08	A
O											
ATOM	302	N	LEU	A	164	266.195	-66.329	104.085	1.00	53.99	A
N											
ATOM	303	CA	LEU	A	164	266.261	-67.732	104.569	1.00	55.36	A
C											
ATOM	304	CB	LEU	A	164	265.516	-68.657	103.598	1.00	54.99	A
C											
ATOM	305	CG	LEU	A	164	264.173	-68.154	103.039	1.00	57.06	A
C											
ATOM	306	CD1	LEU	A	164	264.096	-68.423	101.535	1.00	57.49	A
C											
ATOM	307	CD2	LEU	A	164	263.093	-68.851	103.764	1.00	55.47	A
C											
ATOM	308	C	LEU	A	164	267.715	-68.188	104.665	1.00	52.23	A
C											
ATOM	309	O	LEU	A	164	268.488	-67.990	103.745	1.00	50.98	A
O											

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ATOM    310  N   PHE A 165     268.081 -68.800 105.774  1.00 52.15      A
N
ATOM    311  CA  PHE A 165     269.422 -69.297 105.892  1.00 51.87      A
C
ATOM    312  CB  PHE A 165     269.859 -69.322 107.352  1.00 54.79      A
C
ATOM    313  CG  PHE A 165     270.210 -67.979 107.875  1.00 59.43      A
C
ATOM    314  CD1 PHE A 165     269.232 -67.171 108.426  1.00 61.03      A
C
ATOM    315  CD2 PHE A 165     271.517 -67.493 107.769  1.00 59.15      A
C
ATOM    316  CE1 PHE A 165     269.542 -65.896 108.856  1.00 59.31      A
C
ATOM    317  CE2 PHE A 165     271.835 -66.216 108.196  1.00 59.42      A
C
ATOM    318  CZ  PHE A 165     270.845 -65.412 108.745  1.00 60.41      A
C
ATOM    319  C   PHE A 165     269.598 -70.683 105.287  1.00 52.40      A
C
ATOM    320  O   PHE A 165     268.924 -71.654 105.675  1.00 45.64      A
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ATOM    321  N   LYS A 166     270.504 -70.772 104.320  1.00 52.32      A
N
ATOM    322  CA  LYS A 166     270.786 -72.050 103.696  1.00 53.94      A
C
ATOM    323  CB  LYS A 166     271.911 -71.916 102.708  1.00 47.98      A
C
ATOM    324  CG  LYS A 166     271.540 -71.081 101.498  1.00 41.92      A
C
ATOM    325  CD  LYS A 166     272.530 -71.309 100.383  1.00 38.85      A
C
ATOM    326  CE  LYS A 166     272.490 -70.201  99.345  1.00 31.90      A
C
ATOM    327  NZ  LYS A 166     273.477 -70.401  98.252  1.00 43.47      A
N
ATOM    328  C   LYS A 166     271.159 -73.067 104.740  1.00 51.94      A
C
ATOM    329  O   LYS A 166     270.625 -74.147 104.743  1.00 62.20      A
O
ATOM    330  N   ALA A 167     272.031 -72.699 105.659  1.00 51.64      A
N
ATOM    331  CA  ALA A 167     272.445 -73.632 106.682  1.00 51.81      A
C
ATOM    332  CB  ALA A 167     273.293 -72.935 107.670  1.00 53.31      A
C
ATOM    333  C   ALA A 167     271.234 -74.240 107.369  1.00 53.85      A
C
ATOM    334  O   ALA A 167     271.105 -75.457 107.454  1.00 57.18      A
O
ATOM    335  N   GLN A 168     270.318 -73.403 107.833  1.00 59.28      A
N
ATOM    336  CA  GLN A 168     269.139 -73.902 108.534  1.00 59.95      A
C
ATOM    337  CB  GLN A 168     268.348 -72.736 109.131  1.00 66.12      A
C
ATOM    338  CG  GLN A 168     268.398 -72.648 110.644  1.00 72.61      A
C
ATOM    339  CD  GLN A 168     267.038 -72.270 111.248  1.00 77.64      A
C
ATOM    340  OE1 GLN A 168     266.542 -72.938 112.173  1.00 76.82      A
O
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ATOM    341  NE2 GLN A 168     266.432 -71.196 110.727  1.00 72.17      A
N
ATOM    342  C   GLN A 168     268.221 -74.718 107.635  1.00 55.73      A
C
ATOM    343  O   GLN A 168     267.646 -75.736 108.043  1.00 53.22      A
O
ATOM    344  N   LEU A 169     268.076 -74.262 106.404  1.00 47.44      A
N
ATOM    345  CA  LEU A 169     267.214 -74.954 105.430  1.00 53.18      A
C
ATOM    346  CB  LEU A 169     267.236 -74.247 104.084  1.00 46.05      A
C
ATOM    347  CG  LEU A 169     266.495 -72.939 104.055  1.00 47.35      A
C
ATOM    348  CD1 LEU A 169     266.858 -72.184 102.803  1.00 45.64      A
C
ATOM    349  CD2 LEU A 169     265.005 -73.224 104.130  1.00 44.94      A
C
ATOM    350  C   LEU A 169     267.743 -76.381 105.180  1.00 53.79      A
C
ATOM    351  O   LEU A 169     266.983 -77.361 105.065  1.00 54.87      A
O
ATOM    352  N   GLU A 170     269.057 -76.488 105.056  1.00 54.40      A
N
ATOM    353  CA  GLU A 170     269.692 -77.771 104.839  1.00 58.30      A
C
ATOM    354  CB  GLU A 170     271.162 -77.587 104.678  1.00 57.36      A
C
ATOM    355  CG  GLU A 170     271.585 -77.158 103.319  1.00 66.04      A
C
ATOM    356  CD  GLU A 170     273.099 -76.836 103.260  1.00 73.19      A
C
ATOM    357  OE1 GLU A 170     273.912 -77.755 103.560  1.00 76.86      A
O
ATOM    358  OE2 GLU A 170     273.473 -75.670 102.918  1.00 77.40      A
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ATOM    359  C   GLU A 170     269.481 -78.643 106.045  1.00 60.58      A
C
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O
ATOM    361  N   LYS A 171     269.931 -78.162 107.207  1.00 59.38      A
N
ATOM    362  CA  LYS A 171     269.817 -78.942 108.423  1.00 59.74      A
C
ATOM    363  CB  LYS A 171     270.264 -78.118 109.600  1.00 58.50      A
C
ATOM    364  C   LYS A 171     268.409 -79.500 108.655  1.00 62.87      A
C
ATOM    365  O   LYS A 171     268.227 -80.438 109.441  1.00 65.46      A
O
ATOM    366  N   ALA A 172     267.417 -78.939 107.970  1.00 58.04      A
N
ATOM    367  CA  ALA A 172     266.044 -79.373 108.153  1.00 55.58      A
C
ATOM    368  CB  ALA A 172     265.139 -78.157 108.445  1.00 44.25      A
C
ATOM    369  C   ALA A 172     265.506 -80.129 106.962  1.00 57.83      A
C
ATOM    370  O   ALA A 172     264.406 -80.699 107.038  1.00 63.97      A
O
ATOM    371  N   GLY A 173     266.255 -80.108 105.860  1.00 59.05      A
N
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ATOM	372	CA	GLY	A	173	265.825	-80.806	104.659	1.00	58.57	A
C											
ATOM	373	C	GLY	A	173	264.519	-80.290	104.096	1.00	56.33	A
C											
ATOM	374	O	GLY	A	173	263.636	-81.045	103.722	1.00	57.22	A
O											
ATOM	375	N	VAL	A	174	264.392	-78.983	104.043	1.00	52.27	A
N											
ATOM	376	CA	VAL	A	174	263.183	-78.389	103.520	1.00	51.67	A
C											
ATOM	377	CB	VAL	A	174	262.555	-77.420	104.523	1.00	44.57	A
C											
ATOM	378	CG1	VAL	A	174	262.061	-78.172	105.687	1.00	45.83	A
C											
ATOM	379	CG2	VAL	A	174	263.557	-76.374	104.919	1.00	43.22	A
C											
ATOM	380	C	VAL	A	174	263.518	-77.628	102.230	1.00	55.27	A
C											
ATOM	381	O	VAL	A	174	262.825	-76.679	101.851	1.00	62.81	A
O											
ATOM	382	N	GLU	A	175	264.577	-78.044	101.548	1.00	50.98	A
N											
ATOM	383	CA	GLU	A	175	264.955	-77.393	100.296	1.00	52.00	A
C											
ATOM	384	CB	GLU	A	175	266.251	-77.994	99.721	1.00	47.79	A
C											
ATOM	385	CG	GLU	A	175	267.462	-77.861	100.680	1.00	59.64	A
C											
ATOM	386	CD	GLU	A	175	267.730	-79.101	101.479	1.00	59.83	A
C											
ATOM	387	OE1	GLU	A	175	266.822	-79.948	101.619	1.00	66.12	A
O											
ATOM	388	OE2	GLU	A	175	268.853	-79.219	101.990	1.00	70.43	A
O											
ATOM	389	C	GLU	A	175	263.852	-77.526	99.266	1.00	51.17	A
C											
ATOM	390	O	GLU	A	175	263.637	-76.642	98.463	1.00	57.75	A
O											
ATOM	391	N	HIS	A	176	263.166	-78.661	99.266	1.00	60.20	A
N											
ATOM	392	CA	HIS	A	176	262.080	-78.920	98.312	1.00	61.34	A
C											
ATOM	393	CB	HIS	A	176	261.735	-80.414	98.276	1.00	62.47	A
C											
ATOM	394	CG	HIS	A	176	261.265	-80.959	99.579	1.00	70.92	A
C											
ATOM	395	CD2	HIS	A	176	261.875	-81.020	100.783	1.00	68.70	A
C											
ATOM	396	ND1	HIS	A	176	260.020	-81.533	99.740	1.00	72.07	A
N											
ATOM	397	CE1	HIS	A	176	259.886	-81.925	100.994	1.00	75.43	A
C											
ATOM	398	NE2	HIS	A	176	260.996	-81.625	101.644	1.00	77.22	A
N											
ATOM	399	C	HIS	A	176	260.828	-78.116	98.620	1.00	60.76	A
C											
ATOM	400	O	HIS	A	176	260.058	-77.805	97.733	1.00	64.86	A
O											
ATOM	401	N	GLN	A	177	260.607	-77.784	99.886	1.00	63.60	A
N											
ATOM	402	CA	GLN	A	177	259.436	-76.993	100.239	1.00	59.32	A
C											

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ATOM    403  CB  GLN A 177     259.188 -77.080 101.756  1.00 65.79      A
C
ATOM    404  CG  GLN A 177     258.573 -78.484 102.090  1.00 78.25      A
C
ATOM    405  CD  GLN A 177     258.481 -78.896 103.539  1.00 84.93      A
C
ATOM    406  OE1 GLN A 177     257.670 -79.822 103.897  1.00 89.62      A
O
ATOM    407  NE2 GLN A 177     259.316 -78.274 104.407  1.00 87.76      A
N
ATOM    408  C   GLN A 177     259.647 -75.552  99.730  1.00 54.25      A
C
ATOM    409  O   GLN A 177     258.739 -75.013  99.073  1.00 51.39      A
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ATOM    410  N   LEU A 178     260.844 -74.972  99.942  1.00 45.84      A
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ATOM    411  CA  LEU A 178     261.123 -73.611  99.474  1.00 49.49      A
C
ATOM    412  CB  LEU A 178     262.514 -73.175  99.900  1.00 42.21      A
C
ATOM    413  CG  LEU A 178     263.032 -71.858  99.325  1.00 49.26      A
C
ATOM    414  CD1 LEU A 178     261.981 -70.693  99.584  1.00 37.20      A
C
ATOM    415  CD2 LEU A 178     264.421 -71.557  99.950  1.00 46.43      A
C
ATOM    416  C   LEU A 178     261.030 -73.631  97.939  1.00 46.87      A
C
ATOM    417  O   LEU A 178     260.678 -72.659  97.280  1.00 52.87      A
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ATOM    418  N   ARG A 179     261.314 -74.778  97.360  1.00 52.38      A
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C
ATOM    421  CG  ARG A 179     262.661 -76.085  94.149  1.00 55.19      A
C
ATOM    422  CD  ARG A 179     263.898 -77.002  94.178  1.00 71.41      A
C
ATOM    423  NE  ARG A 179     264.829 -76.685  93.086  1.00 73.48      A
N
ATOM    424  CZ  ARG A 179     264.827 -77.258  91.873  1.00 77.16      A
C
ATOM    425  NH1 ARG A 179     263.941 -78.208  91.565  1.00 70.26      A
N
ATOM    426  NH2 ARG A 179     265.709 -76.874  90.951  1.00 75.62      A
N
ATOM    427  C   ARG A 179     259.841 -74.758  95.383  1.00 46.80      A
C
ATOM    428  O   ARG A 179     259.605 -74.009  94.443  1.00 37.96      A
O
ATOM    429  N   ARG A 180     258.912 -75.494  95.988  1.00 41.56      A
N
ATOM    430  CA  ARG A 180     257.504 -75.451  95.630  1.00 46.45      A
C
ATOM    431  CB  ARG A 180     256.749 -76.543  96.386  1.00 47.01      A
C
ATOM    432  CG  ARG A 180     256.416 -77.762  95.546  1.00 51.52      A
C
ATOM    433  CD  ARG A 180     255.582 -78.783  96.257  1.00 53.97      A
C
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ATOM	434	NE	ARG	A	180	256.374	-79.863	96.824	1.00	69.57	A
N											
ATOM	435	CZ	ARG	A	180	256.902	-79.849	98.046	1.00	76.20	A
C											
ATOM	436	NH1	ARG	A	180	256.721	-78.796	98.846	1.00	85.82	A
N											
ATOM	437	NH2	ARG	A	180	257.614	-80.893	98.475	1.00	82.98	A
N											
ATOM	438	C	ARG	A	180	256.882	-74.100	95.969	1.00	48.19	A
C											
ATOM	439	O	ARG	A	180	256.088	-73.556	95.189	1.00	55.26	A
O											
ATOM	440	N	GLU	A	181	257.235	-73.560	97.130	1.00	49.77	A
N											
ATOM	441	CA	GLU	A	181	256.694	-72.279	97.536	1.00	48.24	A
C											
ATOM	442	CB	GLU	A	181	257.367	-71.820	98.841	1.00	51.28	A
C											
ATOM	443	CG	GLU	A	181	256.969	-70.425	99.303	1.00	55.39	A
C											
ATOM	444	CD	GLU	A	181	257.553	-70.042	100.652	1.00	57.20	A
C											
ATOM	445	OE1	GLU	A	181	258.173	-70.904	101.305	1.00	46.80	A
O											
ATOM	446	OE2	GLU	A	181	257.362	-68.871	101.058	1.00	56.40	A
O											
ATOM	447	C	GLU	A	181	256.958	-71.259	96.430	1.00	49.63	A
C											
ATOM	448	O	GLU	A	181	256.044	-70.571	95.930	1.00	44.79	A
O											
ATOM	449	N	VAL	A	182	258.227	-71.191	96.037	1.00	46.11	A
N											
ATOM	450	CA	VAL	A	182	258.659	-70.228	95.035	1.00	45.55	A
C											
ATOM	451	CB	VAL	A	182	260.183	-70.266	94.833	1.00	40.91	A
C											
ATOM	452	CG1	VAL	A	182	260.560	-69.403	93.678	1.00	38.12	A
C											
ATOM	453	CG2	VAL	A	182	260.875	-69.730	96.059	1.00	51.08	A
C											
ATOM	454	C	VAL	A	182	257.954	-70.443	93.695	1.00	46.82	A
C											
ATOM	455	O	VAL	A	182	257.459	-69.483	93.056	1.00	40.29	A
O											
ATOM	456	N	GLU	A	183	257.936	-71.690	93.237	1.00	48.08	A
N											
ATOM	457	CA	GLU	A	183	257.280	-72.012	91.968	1.00	52.62	A
C											
ATOM	458	CB	GLU	A	183	257.493	-73.478	91.608	1.00	56.60	A
C											
ATOM	459	CG	GLU	A	183	258.695	-73.784	90.808	1.00	70.69	A
C											
ATOM	460	CD	GLU	A	183	258.923	-75.283	90.746	1.00	77.34	A
C											
ATOM	461	OE1	GLU	A	183	257.954	-76.011	90.397	1.00	83.76	A
O											
ATOM	462	OE2	GLU	A	183	260.068	-75.727	91.052	1.00	82.45	A
O											
ATOM	463	C	GLU	A	183	255.800	-71.754	91.912	1.00	49.85	A
C											
ATOM	464	O	GLU	A	183	255.313	-71.138	90.947	1.00	46.36	A
O											

ATOM 465 N ILE A 184 255.098 -72.317 92.898 1.00 46.74 A
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ATOM 466 CA ILE A 184 253.660 -72.157 92.965 1.00 43.86 A
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ATOM 467 CB ILE A 184 253.067 -72.962 94.115 1.00 40.26 A
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ATOM 468 CG2 ILE A 184 251.553 -72.714 94.209 1.00 29.84 A
C
ATOM 469 CG1 ILE A 184 253.313 -74.446 93.860 1.00 36.80 A
C
ATOM 470 CD1 ILE A 184 252.748 -75.369 94.961 1.00 40.80 A
C
ATOM 471 C ILE A 184 253.221 -70.713 93.099 1.00 46.29 A
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ATOM 472 O ILE A 184 252.448 -70.199 92.284 1.00 49.47 A
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ATOM 473 N GLN A 185 253.720 -70.054 94.132 1.00 49.28 A
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ATOM 474 CA GLN A 185 253.328 -68.666 94.388 1.00 52.47 A
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ATOM 475 CB GLN A 185 253.948 -68.189 95.721 1.00 44.73 A
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ATOM 476 CG GLN A 185 253.150 -67.168 96.526 1.00 48.30 A
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ATOM 477 CD GLN A 185 253.861 -66.745 97.745 1.00 54.47 A
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ATOM 478 OE1 GLN A 185 254.700 -67.516 98.331 1.00 61.67 A
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ATOM 479 NE2 GLN A 185 253.553 -65.501 98.201 1.00 56.50 A
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ATOM 480 C GLN A 185 253.707 -67.716 93.231 1.00 50.63 A
C
ATOM 481 O GLN A 185 252.971 -66.780 92.894 1.00 52.61 A
O
ATOM 482 N SER A 186 254.843 -67.972 92.610 1.00 47.27 A
N
ATOM 483 CA SER A 186 255.315 -67.114 91.541 1.00 52.03 A
C
ATOM 484 CB SER A 186 256.692 -67.586 91.048 1.00 51.09 A
C
ATOM 485 OG SER A 186 256.609 -68.877 90.496 1.00 54.11 A
O
ATOM 486 C SER A 186 254.346 -67.050 90.373 1.00 51.30 A
C
ATOM 487 O SER A 186 254.116 -65.999 89.812 1.00 53.71 A
O
ATOM 488 N HIS A 187 253.774 -68.184 90.001 1.00 55.86 A
N
ATOM 489 CA HIS A 187 252.846 -68.233 88.883 1.00 57.28 A
C
ATOM 490 CB HIS A 187 252.945 -69.605 88.190 1.00 68.44 A
C
ATOM 491 CG HIS A 187 254.283 -69.866 87.541 1.00 77.26 A
C
ATOM 492 CD2 HIS A 187 255.147 -69.041 86.892 1.00 78.77 A
C
ATOM 493 ND1 HIS A 187 254.874 -71.114 87.532 1.00 80.45 A
N
ATOM 494 CE1 HIS A 187 256.041 -71.048 86.911 1.00 81.91 A
C
ATOM 495 NE2 HIS A 187 256.232 -69.802 86.512 1.00 81.51 A
N

ATOM	496	C	HIS	A	187	251.418	-67.953	89.300	1.00	57.51	A
C											
ATOM	497	O	HIS	A	187	250.496	-68.154	88.529	1.00	60.26	A
O											
ATOM	498	N	LEU	A	188	251.230	-67.497	90.530	1.00	59.97	A
N											
ATOM	499	CA	LEU	A	188	249.900	-67.189	91.028	1.00	56.67	A
C											
ATOM	500	CB	LEU	A	188	249.832	-67.488	92.511	1.00	57.07	A
C											
ATOM	501	CG	LEU	A	188	248.970	-68.663	92.952	1.00	55.73	A
C											
ATOM	502	CD1	LEU	A	188	249.478	-69.896	92.257	1.00	62.61	A
C											
ATOM	503	CD2	LEU	A	188	249.027	-68.827	94.465	1.00	53.98	A
C											
ATOM	504	C	LEU	A	188	249.598	-65.728	90.777	1.00	57.85	A
C											
ATOM	505	O	LEU	A	188	250.503	-64.881	90.799	1.00	64.49	A
O											
ATOM	506	N	ARG	A	189	248.331	-65.440	90.507	1.00	59.25	A
N											
ATOM	507	CA	ARG	A	189	247.893	-64.067	90.239	1.00	63.66	A
C											
ATOM	508	CB	ARG	A	189	247.927	-63.796	88.734	1.00	64.78	A
C											
ATOM	509	CG	ARG	A	189	249.318	-63.660	88.125	1.00	70.33	A
C											
ATOM	510	CD	ARG	A	189	249.903	-62.285	88.356	1.00	72.14	A
C											
ATOM	511	NE	ARG	A	189	250.864	-61.937	87.301	1.00	81.14	A
N											
ATOM	512	CZ	ARG	A	189	250.716	-60.923	86.432	1.00	82.52	A
C											
ATOM	513	NH1	ARG	A	189	249.636	-60.138	86.478	1.00	79.99	A
N											
ATOM	514	NH2	ARG	A	189	251.658	-60.669	85.521	1.00	82.64	A
N											
ATOM	515	C	ARG	A	189	246.469	-63.844	90.761	1.00	59.43	A
C											
ATOM	516	O	ARG	A	189	245.497	-64.167	90.072	1.00	61.20	A
O											
ATOM	517	N	HIS	A	190	246.342	-63.283	91.964	1.00	56.49	A
N											
ATOM	518	CA	HIS	A	190	245.023	-63.075	92.565	1.00	48.34	A
C											
ATOM	519	CB	HIS	A	190	244.506	-64.377	93.201	1.00	52.70	A
C											
ATOM	520	CG	HIS	A	190	243.036	-64.372	93.489	1.00	49.06	A
C											
ATOM	521	CD2	HIS	A	190	242.038	-65.207	93.107	1.00	52.53	A
C											
ATOM	522	ND1	HIS	A	190	242.449	-63.432	94.302	1.00	51.06	A
N											
ATOM	523	CE1	HIS	A	190	241.155	-63.686	94.414	1.00	46.17	A
C											
ATOM	524	NE2	HIS	A	190	240.878	-64.757	93.697	1.00	43.53	A
N											
ATOM	525	C	HIS	A	190	245.116	-61.998	93.611	1.00	47.54	A
C											
ATOM	526	O	HIS	A	190	246.077	-61.946	94.377	1.00	44.41	A
O											

ATOM	527	N	PRO	A	191	244.119	-61.102	93.645	1.00	49.93	A
N											
ATOM	528	CD	PRO	A	191	242.947	-61.054	92.749	1.00	46.91	A
C											
ATOM	529	CA	PRO	A	191	244.070	-59.992	94.607	1.00	49.33	A
C											
ATOM	530	CB	PRO	A	191	242.694	-59.384	94.346	1.00	50.21	A
C											
ATOM	531	CG	PRO	A	191	242.518	-59.644	92.887	1.00	48.82	A
C											
ATOM	532	C	PRO	A	191	244.239	-60.419	96.072	1.00	46.55	A
C											
ATOM	533	O	PRO	A	191	244.892	-59.719	96.848	1.00	42.94	A
O											
ATOM	534	N	ASN	A	192	243.647	-61.555	96.434	1.00	42.75	A
N											
ATOM	535	CA	ASN	A	192	243.715	-62.060	97.791	1.00	48.46	A
C											
ATOM	536	CB	ASN	A	192	242.378	-62.678	98.192	1.00	45.61	A
C											
ATOM	537	CG	ASN	A	192	241.206	-61.781	97.847	1.00	48.26	A
C											
ATOM	538	OD1	ASN	A	192	240.715	-61.767	96.724	1.00	55.77	A
O											
ATOM	539	ND2	ASN	A	192	240.766	-61.020	98.804	1.00	48.89	A
N											
ATOM	540	C	ASN	A	192	244.831	-63.085	97.953	1.00	44.35	A
C											
ATOM	541	O	ASN	A	192	244.725	-64.017	98.747	1.00	54.33	A
O											
ATOM	542	N	ILE	A	193	245.909	-62.901	97.204	1.00	42.87	A
N											
ATOM	543	CA	ILE	A	193	247.067	-63.781	97.277	1.00	40.40	A
C											
ATOM	544	CB	ILE	A	193	247.054	-64.847	96.138	1.00	40.53	A
C											
ATOM	545	CG2	ILE	A	193	248.292	-65.733	96.243	1.00	22.41	A
C											
ATOM	546	CG1	ILE	A	193	245.800	-65.732	96.274	1.00	36.30	A
C											
ATOM	547	CD1	ILE	A	193	245.709	-66.793	95.246	1.00	46.23	A
C											
ATOM	548	C	ILE	A	193	248.330	-62.944	97.180	1.00	43.53	A
C											
ATOM	549	O	ILE	A	193	248.481	-62.176	96.228	1.00	41.20	A
O											
ATOM	550	N	LEU	A	194	249.217	-63.070	98.171	1.00	46.32	A
N											
ATOM	551	CA	LEU	A	194	250.449	-62.307	98.168	1.00	48.93	A
C											
ATOM	552	CB	LEU	A	194	251.233	-62.511	99.477	1.00	44.51	A
C											
ATOM	553	CG	LEU	A	194	252.485	-61.630	99.579	1.00	41.08	A
C											
ATOM	554	CD1	LEU	A	194	252.055	-60.195	99.956	1.00	43.64	A
C											
ATOM	555	CD2	LEU	A	194	253.437	-62.183	100.655	1.00	41.05	A
C											
ATOM	556	C	LEU	A	194	251.290	-62.773	96.988	1.00	49.00	A
C											
ATOM	557	O	LEU	A	194	251.553	-63.975	96.826	1.00	53.77	A
O											

ATOM	558	N	ARG	A	195	251.712	-61.823	96.162	1.00	43.08	A
N											
ATOM	559	CA	ARG	A	195	252.553	-62.166	95.023	1.00	45.19	A
C											
ATOM	560	CB	ARG	A	195	252.509	-61.043	93.969	1.00	43.15	A
C											
ATOM	561	CG	ARG	A	195	251.180	-60.913	93.213	1.00	46.56	A
C											
ATOM	562	CD	ARG	A	195	251.400	-60.798	91.730	1.00	59.57	A
C											
ATOM	563	NE	ARG	A	195	252.816	-60.787	91.377	1.00	72.51	A
N											
ATOM	564	CZ	ARG	A	195	253.288	-60.716	90.133	1.00	78.66	A
C											
ATOM	565	NH1	ARG	A	195	252.446	-60.646	89.119	1.00	80.03	A
N											
ATOM	566	NH2	ARG	A	195	254.603	-60.723	89.898	1.00	82.29	A
N											
ATOM	567	C	ARG	A	195	254.004	-62.450	95.390	1.00	44.60	A
C											
ATOM	568	O	ARG	A	195	254.470	-62.001	96.429	1.00	47.11	A
O											
ATOM	569	N	LEU	A	196	254.710	-63.177	94.522	1.00	48.18	A
N											
ATOM	570	CA	LEU	A	196	256.116	-63.465	94.735	1.00	48.30	A
C											
ATOM	571	CB	LEU	A	196	256.345	-64.954	95.048	1.00	50.39	A
C											
ATOM	572	CG	LEU	A	196	257.768	-65.343	95.383	1.00	41.45	A
C											
ATOM	573	CD1	LEU	A	196	258.090	-64.804	96.698	1.00	58.09	A
C											
ATOM	574	CD2	LEU	A	196	257.886	-66.788	95.411	1.00	44.21	A
C											
ATOM	575	C	LEU	A	196	256.799	-63.091	93.432	1.00	50.04	A
C											
ATOM	576	O	LEU	A	196	256.887	-63.926	92.532	1.00	56.48	A
O											
ATOM	577	N	TYR	A	197	257.301	-61.854	93.359	1.00	52.17	A
N											
ATOM	578	CA	TYR	A	197	257.970	-61.330	92.172	1.00	49.64	A
C											
ATOM	579	CB	TYR	A	197	258.419	-59.908	92.460	1.00	44.72	A
C											
ATOM	580	CG	TYR	A	197	257.289	-59.034	92.959	1.00	43.03	A
C											
ATOM	581	CD1	TYR	A	197	257.445	-58.246	94.117	1.00	44.46	A
C											
ATOM	582	CE1	TYR	A	197	256.439	-57.433	94.583	1.00	51.15	A
C											
ATOM	583	CD2	TYR	A	197	256.085	-58.978	92.278	1.00	41.30	A
C											
ATOM	584	CE2	TYR	A	197	255.057	-58.161	92.730	1.00	50.46	A
C											
ATOM	585	CZ	TYR	A	197	255.243	-57.390	93.887	1.00	52.65	A
C											
ATOM	586	OH	TYR	A	197	254.234	-56.573	94.338	1.00	63.16	A
O											
ATOM	587	C	TYR	A	197	259.142	-62.186	91.684	1.00	51.16	A
C											
ATOM	588	O	TYR	A	197	259.129	-62.683	90.572	1.00	58.21	A
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ATOM    589  N   GLY A 198     260.141 -62.378  92.529  1.00 53.24      A
N
ATOM    590  CA  GLY A 198     261.296 -63.164  92.148  1.00 47.33      A
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ATOM    591  C   GLY A 198     262.028 -63.697  93.360  1.00 48.93      A
C
ATOM    592  O   GLY A 198     261.447 -63.928  94.412  1.00 49.80      A
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ATOM    593  N   TYR A 199     263.316 -63.941  93.204  1.00 48.77      A
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ATOM    594  CA  TYR A 199     264.134 -64.436  94.315  1.00 50.98      A
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ATOM    595  CB  TYR A 199     263.712 -65.834  94.699  1.00 54.11      A
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ATOM    596  CG  TYR A 199     264.323 -66.921  93.853  1.00 56.57      A
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ATOM    597  CD1 TYR A 199     265.506 -67.521  94.238  1.00 57.21      A
C
ATOM    598  CE1 TYR A 199     266.088 -68.526  93.471  1.00 58.18      A
C
ATOM    599  CD2 TYR A 199     263.715 -67.351  92.664  1.00 59.67      A
C
ATOM    600  CE2 TYR A 199     264.286 -68.349  91.899  1.00 59.17      A
C
ATOM    601  CZ  TYR A 199     265.479 -68.933  92.308  1.00 59.36      A
C
ATOM    602  OH  TYR A 199     266.075 -69.917  91.535  1.00 63.54      A
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ATOM    603  C   TYR A 199     265.563 -64.463  93.826  1.00 48.41      A
C
ATOM    604  O   TYR A 199     265.787 -64.357  92.640  1.00 47.41      A
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ATOM    605  N   PHE A 200     266.542 -64.591  94.701  1.00 43.25      A
N
ATOM    606  CA  PHE A 200     267.921 -64.582  94.221  1.00 40.67      A
C
ATOM    607  CB  PHE A 200     268.427 -63.159  93.950  1.00 43.34      A
C
ATOM    608  CG  PHE A 200     268.272 -62.218  95.134  1.00 48.79      A
C
ATOM    609  CD1 PHE A 200     269.249 -62.115  96.166  1.00 50.06      A
C
ATOM    610  CD2 PHE A 200     267.178 -61.322  95.162  1.00 52.88      A
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ATOM    611  CE1 PHE A 200     269.107 -61.097  97.192  1.00 53.41      A
C
ATOM    612  CE2 PHE A 200     267.048 -60.331  96.166  1.00 49.85      A
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ATOM    613  CZ  PHE A 200     267.993 -60.201  97.160  1.00 49.27      A
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ATOM    614  C   PHE A 200     268.645 -65.113  95.325  1.00 47.09      A
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ATOM    615  O   PHE A 200     268.037 -65.599  96.262  1.00 47.13      A
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ATOM    616  N   HIS A 201     269.953 -65.125  95.219  1.00 56.46      A
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ATOM    617  CA  HIS A 201     270.635 -65.604  96.382  1.00 56.94      A
C
ATOM    618  CB  HIS A 201     270.242 -67.052  96.679  1.00 62.89      A
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ATOM    619  CG  HIS A 201     270.668 -68.030  95.648  1.00 66.27      A
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ATOM    620  CD2 HIS A 201     270.131 -68.454  94.469  1.00 68.86      A
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ATOM    621  ND1 HIS A 201     271.876 -68.658  95.778  1.00 70.42      A
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ATOM    622  CE1 HIS A 201     272.086 -69.425  94.727  1.00 63.77      A
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ATOM    623  NE2 HIS A 201     271.048 -69.319  93.917  1.00 69.53      A
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ATOM    624  C   HIS A 201     272.082 -65.339  96.531  1.00 59.01      A
C
ATOM    625  O   HIS A 201     272.657 -64.604  95.737  1.00 56.46      A
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ATOM    626  N   ASP A 202     272.636 -65.783  97.652  1.00 53.50      A
N
ATOM    627  CA  ASP A 202     274.052 -65.546  97.850  1.00 58.12      A
C
ATOM    628  CB  ASP A 202     274.321 -64.225  98.617  1.00 61.13      A
C
ATOM    629  CG  ASP A 202     273.888 -64.255 100.090  1.00 65.37      A
C
ATOM    630  OD1 ASP A 202     273.969 -65.308 100.803  1.00 69.09      A
O
ATOM    631  OD2 ASP A 202     273.489 -63.181 100.569  1.00 73.25      A
O
ATOM    632  C   ASP A 202     274.782 -66.745  98.522  1.00 59.73      A
C
ATOM    633  O   ASP A 202     274.357 -67.899  98.426  1.00 61.93      A
O
ATOM    634  N   ALA A 203     275.910 -66.473  99.163  1.00 59.60      A
N
ATOM    635  CA  ALA A 203     276.705 -67.507  99.793  1.00 59.87      A
C
ATOM    636  CB  ALA A 203     278.079 -66.933 100.191  1.00 57.31      A
C
ATOM    637  C   ALA A 203     276.068 -68.138 100.990  1.00 60.08      A
C
ATOM    638  O   ALA A 203     276.287 -69.294 101.229  1.00 62.79      A
O
ATOM    639  N   THR A 204     275.291 -67.377 101.748  1.00 60.13      A
N
ATOM    640  CA  THR A 204     274.700 -67.893 102.968  1.00 58.14      A
C
ATOM    641  CB  THR A 204     275.067 -67.010 104.168  1.00 54.92      A
C
ATOM    642  OG1 THR A 204     275.068 -65.622 103.799  1.00 51.82      A
O
ATOM    643  CG2 THR A 204     276.406 -67.388 104.681  1.00 55.25      A
C
ATOM    644  C   THR A 204     273.203 -68.070 102.993  1.00 61.74      A
C
ATOM    645  O   THR A 204     272.662 -69.063 103.547  1.00 66.23      A
O
ATOM    646  N   ARG A 205     272.517 -67.099 102.434  1.00 58.56      A
N
ATOM    647  CA  ARG A 205     271.091 -67.217 102.444  1.00 58.96      A
C
ATOM    648  CB  ARG A 205     270.505 -66.287 103.493  1.00 56.07      A
C
ATOM    649  CG  ARG A 205     270.986 -64.877 103.382  1.00 59.74      A
C
ATOM    650  CD  ARG A 205     271.764 -64.493 104.616  1.00 62.84      A
C
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ATOM	651	NE	ARG	A	205	272.739	-63.462	104.285	1.00	73.59	A
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ATOM	652	CZ	ARG	A	205	273.407	-62.747	105.185	1.00	79.55	A
C											
ATOM	653	NH1	ARG	A	205	273.198	-62.946	106.482	1.00	80.70	A
N											
ATOM	654	NH2	ARG	A	205	274.297	-61.845	104.792	1.00	87.21	A
N											
ATOM	655	C	ARG	A	205	270.418	-67.012	101.120	1.00	56.37	A
C											
ATOM	656	O	ARG	A	205	271.034	-66.604	100.116	1.00	64.50	A
O											
ATOM	657	N	VAL	A	206	269.150	-67.373	101.124	1.00	54.49	A
N											
ATOM	658	CA	VAL	A	206	268.304	-67.238	99.960	1.00	50.29	A
C											
ATOM	659	CB	VAL	A	206	267.536	-68.522	99.670	1.00	47.01	A
C											
ATOM	660	CG1	VAL	A	206	266.800	-68.370	98.374	1.00	38.39	A
C											
ATOM	661	CG2	VAL	A	206	268.488	-69.696	99.620	1.00	42.93	A
C											
ATOM	662	C	VAL	A	206	267.306	-66.124	100.321	1.00	50.23	A
C											
ATOM	663	O	VAL	A	206	266.870	-65.982	101.487	1.00	49.82	A
O											
ATOM	664	N	TYR	A	207	266.958	-65.330	99.320	1.00	47.64	A
N											
ATOM	665	CA	TYR	A	207	266.053	-64.226	99.517	1.00	47.19	A
C											
ATOM	666	CB	TYR	A	207	266.748	-62.879	99.204	1.00	44.49	A
C											
ATOM	667	CG	TYR	A	207	268.077	-62.684	99.852	1.00	52.24	A
C											
ATOM	668	CD1	TYR	A	207	269.198	-63.362	99.385	1.00	51.97	A
C											
ATOM	669	CE1	TYR	A	207	270.438	-63.194	99.978	1.00	60.89	A
C											
ATOM	670	CD2	TYR	A	207	268.227	-61.820	100.938	1.00	55.49	A
C											
ATOM	671	CE2	TYR	A	207	269.499	-61.638	101.553	1.00	62.31	A
C											
ATOM	672	CZ	TYR	A	207	270.583	-62.327	101.069	1.00	60.88	A
C											
ATOM	673	OH	TYR	A	207	271.783	-62.141	101.704	1.00	68.24	A
O											
ATOM	674	C	TYR	A	207	264.837	-64.374	98.618	1.00	42.31	A
C											
ATOM	675	O	TYR	A	207	264.940	-64.704	97.438	1.00	43.03	A
O											
ATOM	676	N	LEU	A	208	263.671	-64.078	99.171	1.00	47.18	A
N											
ATOM	677	CA	LEU	A	208	262.441	-64.129	98.377	1.00	49.66	A
C											
ATOM	678	CB	LEU	A	208	261.411	-65.084	99.005	1.00	50.68	A
C											
ATOM	679	CG	LEU	A	208	261.731	-66.573	98.967	1.00	50.97	A
C											
ATOM	680	CD1	LEU	A	208	260.525	-67.349	99.471	1.00	51.61	A
C											
ATOM	681	CD2	LEU	A	208	262.019	-66.964	97.575	1.00	53.77	A
C											

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ATOM    682  C   LEU A 208     261.849 -62.733  98.264  1.00 50.25      A
C
ATOM    683  O   LEU A 208     261.525 -62.085  99.278  1.00 54.78      A
O
ATOM    684  N   ILE A 209     261.692 -62.286  97.027  1.00 50.37      A
N
ATOM    685  CA  ILE A 209     261.154 -60.971  96.752  1.00 49.74      A
C
ATOM    686  CB  ILE A 209     261.695 -60.499  95.420  1.00 50.44      A
C
ATOM    687  CG2 ILE A 209     261.168 -59.096  95.082  1.00 50.97      A
C
ATOM    688  CG1 ILE A 209     263.225 -60.485  95.511  1.00 49.66      A
C
ATOM    689  CD1 ILE A 209     263.919 -60.607  94.181  1.00 51.66      A
C
ATOM    690  C   ILE A 209     259.624 -61.075  96.749  1.00 51.17      A
C
ATOM    691  O   ILE A 209     259.048 -61.543  95.755  1.00 54.45      A
O
ATOM    692  N   LEU A 210     258.981 -60.655  97.854  1.00 47.03      A
N
ATOM    693  CA  LEU A 210     257.530 -60.728  97.990  1.00 43.40      A
C
ATOM    694  CB  LEU A 210     257.164 -61.286  99.362  1.00 43.91      A
C
ATOM    695  CG  LEU A 210     257.762 -62.625  99.773  1.00 42.46      A
C
ATOM    696  CD1 LEU A 210     257.695 -62.764 101.264  1.00 44.44      A
C
ATOM    697  CD2 LEU A 210     257.029 -63.701  99.100  1.00 44.23      A
C
ATOM    698  C   LEU A 210     256.873 -59.393  97.827  1.00 42.69      A
C
ATOM    699  O   LEU A 210     257.528 -58.371  97.627  1.00 50.83      A
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ATOM    700  N   GLU A 211     255.552 -59.403  97.901  1.00 45.93      A
N
ATOM    701  CA  GLU A 211     254.757 -58.173  97.813  1.00 41.90      A
C
ATOM    702  CB  GLU A 211     253.383 -58.471  97.201  1.00 39.85      A
C
ATOM    703  CG  GLU A 211     252.402 -57.354  97.290  1.00 41.17      A
C
ATOM    704  CD  GLU A 211     250.976 -57.788  96.890  1.00 51.54      A
C
ATOM    705  OE1 GLU A 211     250.012 -56.980  97.025  1.00 57.54      A
O
ATOM    706  OE2 GLU A 211     250.798 -58.950  96.438  1.00 52.59      A
O
ATOM    707  C   GLU A 211     254.608 -57.669  99.259  1.00 38.67      A
C
ATOM    708  O   GLU A 211     254.507 -58.477 100.200  1.00 42.39      A
O
ATOM    709  N   TYR A 212     254.619 -56.346  99.428  1.00 43.63      A
N
ATOM    710  CA  TYR A 212     254.500 -55.725 100.757  1.00 47.96      A
C
ATOM    711  CB  TYR A 212     255.181 -54.338 100.753  1.00 46.03      A
C
ATOM    712  CG  TYR A 212     255.029 -53.534 102.025  1.00 44.95      A
C
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C
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C
ATOM    715  CD2 TYR A 212     254.639 -52.193 101.984  1.00 44.86      A
C
ATOM    716  CE2 TYR A 212     254.473 -51.424 103.164  1.00 50.04      A
C
ATOM    717  CZ  TYR A 212     254.693 -52.019 104.372  1.00 48.45      A
C
ATOM    718  OH  TYR A 212     254.523 -51.276 105.514  1.00 53.45      A
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ATOM    719  C   TYR A 212     253.041 -55.618 101.248  1.00 50.57      A
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ATOM    720  O   TYR A 212     252.153 -55.140 100.508  1.00 51.02      A
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ATOM    722  CA  ALA A 213     251.459 -56.040 103.078  1.00 51.96      A
C
ATOM    723  CB  ALA A 213     251.084 -57.386 103.656  1.00 42.77      A
C
ATOM    724  C   ALA A 213     251.528 -54.973 104.177  1.00 46.25      A
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ATOM    725  O   ALA A 213     251.958 -55.259 105.280  1.00 57.39      A
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ATOM    726  N   PRO A 214     251.109 -53.734 103.869  1.00 45.44      A
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ATOM    727  CD  PRO A 214     250.592 -53.315 102.549  1.00 45.81      A
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ATOM    728  CA  PRO A 214     251.118 -52.597 104.782  1.00 37.64      A
C
ATOM    729  CB  PRO A 214     250.400 -51.512 103.991  1.00 44.41      A
C
ATOM    730  CG  PRO A 214     250.755 -51.821 102.584  1.00 45.51      A
C
ATOM    731  C   PRO A 214     250.481 -52.833 106.112  1.00 39.63      A
C
ATOM    732  O   PRO A 214     251.116 -52.486 107.123  1.00 38.67      A
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ATOM    733  N   LEU A 215     249.287 -53.446 106.124  1.00 33.01      A
N
ATOM    734  CA  LEU A 215     248.570 -53.617 107.371  1.00 35.54      A
C
ATOM    735  CB  LEU A 215     247.074 -53.585 107.083  1.00 39.80      A
C
ATOM    736  CG  LEU A 215     246.571 -52.332 106.331  1.00 39.22      A
C
ATOM    737  CD1 LEU A 215     245.025 -52.236 106.407  1.00 37.56      A
C
ATOM    738  CD2 LEU A 215     247.156 -51.166 106.898  1.00 36.39      A
C
ATOM    739  C   LEU A 215     248.923 -54.805 108.248  1.00 43.21      A
C
ATOM    740  O   LEU A 215     248.208 -55.121 109.220  1.00 39.03      A
O
ATOM    741  N   GLY A 216     250.022 -55.466 107.906  1.00 42.62      A
N
ATOM    742  CA  GLY A 216     250.443 -56.630 108.669  1.00 46.42      A
C
ATOM    743  C   GLY A 216     249.594 -57.891 108.554  1.00 44.15      A
C
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ATOM	744	O	GLY	A	216	248.995	-58.166	107.504	1.00	46.45	A
O											
ATOM	745	N	THR	A	217	249.523	-58.640	109.656	1.00	39.98	A
N											
ATOM	746	CA	THR	A	217	248.774	-59.889	109.669	1.00	43.21	A
C											
ATOM	747	CB	THR	A	217	249.583	-61.040	110.286	1.00	43.67	A
C											
ATOM	748	OG1	THR	A	217	249.791	-60.782	111.678	1.00	51.00	A
O											
ATOM	749	CG2	THR	A	217	250.905	-61.201	109.605	1.00	41.04	A
C											
ATOM	750	C	THR	A	217	247.450	-59.858	110.416	1.00	42.99	A
C											
ATOM	751	O	THR	A	217	247.185	-58.962	111.227	1.00	41.59	A
O											
ATOM	752	N	VAL	A	218	246.646	-60.881	110.166	1.00	41.73	A
N											
ATOM	753	CA	VAL	A	218	245.335	-61.037	110.766	1.00	41.12	A
C											
ATOM	754	CB	VAL	A	218	244.564	-62.091	109.970	1.00	41.84	A
C											
ATOM	755	CG1	VAL	A	218	243.170	-62.251	110.488	1.00	43.61	A
C											
ATOM	756	CG2	VAL	A	218	244.544	-61.670	108.463	1.00	33.71	A
C											
ATOM	757	C	VAL	A	218	245.610	-61.486	112.201	1.00	40.94	A
C											
ATOM	758	O	VAL	A	218	244.789	-61.326	113.078	1.00	51.00	A
O											
ATOM	759	N	TYR	A	219	246.801	-62.026	112.429	1.00	45.88	A
N											
ATOM	760	CA	TYR	A	219	247.233	-62.484	113.757	1.00	42.54	A
C											
ATOM	761	CB	TYR	A	219	248.607	-63.148	113.673	1.00	45.91	A
C											
ATOM	762	CG	TYR	A	219	249.102	-63.676	115.011	1.00	46.80	A
C											
ATOM	763	CD1	TYR	A	219	248.755	-64.925	115.464	1.00	45.83	A
C											
ATOM	764	CE1	TYR	A	219	249.176	-65.377	116.693	1.00	53.23	A
C											
ATOM	765	CD2	TYR	A	219	249.884	-62.892	115.825	1.00	46.38	A
C											
ATOM	766	CE2	TYR	A	219	250.310	-63.314	117.053	1.00	52.61	A
C											
ATOM	767	CZ	TYR	A	219	249.961	-64.565	117.510	1.00	53.76	A
C											
ATOM	768	OH	TYR	A	219	250.361	-64.985	118.789	1.00	54.10	A
O											
ATOM	769	C	TYR	A	219	247.323	-61.287	114.702	1.00	44.93	A
C											
ATOM	770	O	TYR	A	219	246.745	-61.322	115.825	1.00	40.09	A
O											
ATOM	771	N	ARG	A	220	248.031	-60.243	114.240	1.00	37.14	A
N											
ATOM	772	CA	ARG	A	220	248.172	-59.035	115.029	1.00	44.63	A
C											
ATOM	773	CB	ARG	A	220	249.213	-58.086	114.396	1.00	42.95	A
C											
ATOM	774	C	ARG	A	220	246.828	-58.318	115.225	1.00	43.95	A
C											

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ATOM    775  O   ARG A 220     246.563 -57.773 116.314  1.00 44.55      A
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ATOM    776  N   GLU A 221     245.973 -58.369 114.198  1.00 44.85      A
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ATOM    777  CA  GLU A 221     244.688 -57.692 114.255  1.00 43.30      A
C
ATOM    778  CB  GLU A 221     244.031 -57.678 112.884  1.00 46.86      A
C
ATOM    779  CG  GLU A 221     242.921 -56.648 112.713  1.00 56.65      A
C
ATOM    780  CD  GLU A 221     243.442 -55.193 112.758  1.00 63.09      A
C
ATOM    781  OE1 GLU A 221     242.629 -54.238 112.637  1.00 66.10      A
O
ATOM    782  OE2 GLU A 221     244.670 -55.005 112.919  1.00 66.07      A
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ATOM    783  C   GLU A 221     243.806 -58.412 115.243  1.00 46.56      A
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ATOM    784  O   GLU A 221     242.959 -57.802 115.900  1.00 44.66      A
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ATOM    785  N   LEU A 222     244.028 -59.719 115.362  1.00 46.74      A
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ATOM    786  CA  LEU A 222     243.259 -60.550 116.272  1.00 40.98      A
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ATOM    787  CB  LEU A 222     243.444 -62.013 115.880  1.00 42.79      A
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ATOM    788  CG  LEU A 222     242.339 -62.985 116.313  1.00 48.20      A
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ATOM    789  CD1 LEU A 222     240.982 -62.509 115.826  1.00 42.35      A
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ATOM    790  CD2 LEU A 222     242.649 -64.361 115.761  1.00 47.96      A
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ATOM    791  C   LEU A 222     243.744 -60.292 117.718  1.00 45.64      A
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ATOM    792  O   LEU A 222     242.995 -60.390 118.692  1.00 46.35      A
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ATOM    793  N   GLN A 223     245.008 -59.938 117.875  1.00 47.19      A
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ATOM    794  CA  GLN A 223     245.539 -59.670 119.203  1.00 48.16      A
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ATOM    795  CB  GLN A 223     247.056 -59.584 119.112  1.00 49.22      A
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ATOM    796  CG  GLN A 223     247.819 -60.926 119.032  1.00 56.96      A
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ATOM    797  CD  GLN A 223     249.300 -60.732 118.879  1.00 66.12      A
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ATOM    799  NE2 GLN A 223     250.067 -61.453 119.755  1.00 65.96      A
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ATOM    802  N   LYS A 224     244.877 -57.398 118.779  1.00 53.43      A
N
ATOM    803  CA  LYS A 224     244.412 -56.042 119.021  1.00 52.16      A
C
ATOM    804  CB  LYS A 224     244.668 -55.276 117.729  1.00 51.41      A
C
ATOM    805  CG  LYS A 224     244.740 -53.805 117.796  1.00 58.82      A
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ATOM    806  CD  LYS A 224     245.109 -53.234 116.429  1.00 58.34      A
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ATOM    807  CE  LYS A 224     244.105 -52.175 115.957  1.00 57.11      A
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ATOM    808  NZ  LYS A 224     243.509 -52.549 114.632  1.00 62.05      A
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ATOM    809  C   LYS A 224     242.909 -55.999 119.415  1.00 46.25      A
C
ATOM    810  O   LYS A 224     242.551 -55.374 120.392  1.00 53.53      A
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ATOM    811  N   LEU A 225     242.054 -56.685 118.658  1.00 40.03      A
N
ATOM    812  CA  LEU A 225     240.616 -56.712 118.885  1.00 28.18      A
C
ATOM    813  CB  LEU A 225     239.918 -56.682 117.544  1.00 32.03      A
C
ATOM    814  CG  LEU A 225     240.538 -55.704 116.515  1.00 37.72      A
C
ATOM    815  CD1 LEU A 225     239.725 -55.736 115.208  1.00 28.64      A
C
ATOM    816  CD2 LEU A 225     240.577 -54.252 117.096  1.00 32.47      A
C
ATOM    817  C   LEU A 225     240.076 -57.907 119.686  1.00 39.70      A
C
ATOM    818  O   LEU A 225     238.896 -57.954 120.056  1.00 27.45      A
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ATOM    819  N   SER A 226     240.939 -58.877 119.958  1.00 33.23      A
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ATOM    820  CA  SER A 226     240.528 -60.051 120.695  1.00 38.91      A
C
ATOM    821  CB  SER A 226     239.864 -59.653 122.015  1.00 42.93      A
C
ATOM    822  OG  SER A 226     240.536 -58.570 122.642  1.00 59.01      A
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ATOM    823  C   SER A 226     239.548 -60.869 119.867  1.00 40.96      A
C
ATOM    824  O   SER A 226     239.777 -62.029 119.592  1.00 45.01      A
O
ATOM    825  N   LYS A 227     238.433 -60.270 119.484  1.00 43.12      A
N
ATOM    826  CA  LYS A 227     237.409 -60.968 118.693  1.00 37.87      A
C
ATOM    827  CB  LYS A 227     236.160 -61.246 119.551  1.00 41.34      A
C
ATOM    828  CG  LYS A 227     236.384 -62.150 120.650  1.00 49.95      A
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ATOM    829  CD  LYS A 227     235.126 -62.365 121.469  1.00 59.51      A
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ATOM    830  CE  LYS A 227     234.854 -61.186 122.468  1.00 64.97      A
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ATOM    831  NZ  LYS A 227     234.813 -61.628 123.907  1.00 64.50      A
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ATOM    832  C   LYS A 227     237.009 -60.044 117.520  1.00 37.96      A
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ATOM    833  O   LYS A 227     237.061 -58.799 117.619  1.00 40.95      A
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ATOM    834  N   PHE A 228     236.575 -60.655 116.431  1.00 34.94      A
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ATOM    835  CA  PHE A 228     236.175 -59.917 115.262  1.00 34.74      A
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ATOM    836  CB  PHE A 228     236.793 -60.534 113.998  1.00 34.85      A
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ATOM 837 CG PHE A 228 238.248 -60.293 113.849 1.00 43.10 A
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ATOM 838 CD1 PHE A 228 238.975 -61.009 112.913 1.00 43.37 A
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ATOM 839 CD2 PHE A 228 238.899 -59.395 114.656 1.00 38.38 A
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ATOM 840 CE1 PHE A 228 240.341 -60.832 112.796 1.00 48.51 A
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ATOM 841 CE2 PHE A 228 240.266 -59.207 114.554 1.00 47.20 A
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ATOM 842 CZ PHE A 228 240.999 -59.919 113.631 1.00 48.16 A
C
ATOM 843 C PHE A 228 234.654 -60.063 115.208 1.00 40.38 A
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ATOM 844 O PHE A 228 234.102 -61.082 115.664 1.00 36.38 A
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ATOM 845 N ASP A 229 233.963 -59.053 114.687 1.00 40.55 A
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ATOM 846 CA ASP A 229 232.525 -59.184 114.534 1.00 38.86 A
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ATOM 847 CB ASP A 229 231.823 -57.832 114.440 1.00 49.26 A
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ATOM 848 CG ASP A 229 232.394 -56.912 113.357 1.00 51.97 A
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ATOM 849 OD1 ASP A 229 232.396 -57.278 112.179 1.00 54.02 A
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ATOM 850 OD2 ASP A 229 232.806 -55.788 113.699 1.00 55.60 A
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ATOM 851 C ASP A 229 232.180 -60.027 113.304 1.00 41.70 A
C
ATOM 852 O ASP A 229 233.039 -60.366 112.480 1.00 35.62 A
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ATOM 853 N GLU A 230 230.905 -60.365 113.193 1.00 40.43 A
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ATOM 854 CA GLU A 230 230.434 -61.213 112.114 1.00 43.61 A
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ATOM 855 CB GLU A 230 228.939 -61.526 112.298 1.00 43.33 A
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ATOM 856 CG GLU A 230 228.630 -62.147 113.653 1.00 43.90 A
C
ATOM 857 CD GLU A 230 227.292 -62.967 113.627 1.00 48.51 A
C
ATOM 858 OE1 GLU A 230 226.230 -62.374 113.308 1.00 37.93 A
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ATOM 859 OE2 GLU A 230 227.300 -64.204 113.916 1.00 42.11 A
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ATOM 860 C GLU A 230 230.661 -60.546 110.778 1.00 43.16 A
C
ATOM 861 O GLU A 230 230.878 -61.205 109.779 1.00 50.29 A
O
ATOM 862 N GLN A 231 230.590 -59.225 110.748 1.00 49.18 A
N
ATOM 863 CA GLN A 231 230.742 -58.501 109.489 1.00 49.70 A
C
ATOM 864 CB GLN A 231 230.311 -57.029 109.685 1.00 57.14 A
C
ATOM 865 CG GLN A 231 229.958 -56.236 108.412 1.00 62.54 A
C
ATOM 866 CD GLN A 231 231.200 -55.770 107.642 1.00 71.69 A
C
ATOM 867 OE1 GLN A 231 232.065 -55.042 108.191 1.00 72.68 A
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ATOM	868	NE2	GLN	A	231	231.300	-56.184	106.359	1.00	72.33	A
N											
ATOM	869	C	GLN	A	231	232.197	-58.614	109.018	1.00	45.76	A
C											
ATOM	870	O	GLN	A	231	232.470	-58.874	107.846	1.00	46.46	A
O											
ATOM	871	N	ARG	A	232	233.131	-58.437	109.949	1.00	43.95	A
N											
ATOM	872	CA	ARG	A	232	234.560	-58.503	109.661	1.00	38.33	A
C											
ATOM	873	CB	ARG	A	232	235.365	-57.998	110.861	1.00	39.16	A
C											
ATOM	874	CG	ARG	A	232	236.867	-58.073	110.703	1.00	31.46	A
C											
ATOM	875	CD	ARG	A	232	237.514	-57.172	111.705	1.00	51.25	A
C											
ATOM	876	NE	ARG	A	232	238.871	-56.815	111.334	1.00	58.24	A
N											
ATOM	877	CZ	ARG	A	232	239.275	-55.581	111.111	1.00	65.45	A
C											
ATOM	878	NH1	ARG	A	232	238.395	-54.594	111.226	1.00	62.94	A
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ATOM	879	NH2	ARG	A	232	240.551	-55.369	110.780	1.00	72.17	A
N											
ATOM	880	C	ARG	A	232	234.950	-59.946	109.369	1.00	42.02	A
C											
ATOM	881	O	ARG	A	232	235.757	-60.183	108.517	1.00	45.04	A
O											
ATOM	882	N	THR	A	233	234.372	-60.909	110.084	1.00	43.50	A
N											
ATOM	883	CA	THR	A	233	234.697	-62.320	109.891	1.00	37.00	A
C											
ATOM	884	CB	THR	A	233	234.104	-63.175	110.992	1.00	35.89	A
C											
ATOM	885	OG1	THR	A	233	234.543	-62.696	112.268	1.00	30.74	A
O											
ATOM	886	CG2	THR	A	233	234.488	-64.641	110.763	1.00	22.73	A
C											
ATOM	887	C	THR	A	233	234.149	-62.834	108.555	1.00	45.73	A
C											
ATOM	888	O	THR	A	233	234.857	-63.523	107.844	1.00	45.99	A
O											
ATOM	889	N	ALA	A	234	232.892	-62.501	108.228	1.00	44.83	A
N											
ATOM	890	CA	ALA	A	234	232.256	-62.897	106.960	1.00	41.77	A
C											
ATOM	891	CB	ALA	A	234	230.852	-62.351	106.893	1.00	39.48	A
C											
ATOM	892	C	ALA	A	234	233.064	-62.395	105.744	1.00	44.77	A
C											
ATOM	893	O	ALA	A	234	233.273	-63.131	104.786	1.00	39.69	A
O											
ATOM	894	N	THR	A	235	233.543	-61.155	105.799	1.00	43.07	A
N											
ATOM	895	CA	THR	A	235	234.328	-60.579	104.722	1.00	44.31	A
C											
ATOM	896	CB	THR	A	235	234.557	-59.058	104.926	1.00	44.88	A
C											
ATOM	897	OG1	THR	A	235	233.306	-58.373	104.984	1.00	49.29	A
O											
ATOM	898	CG2	THR	A	235	235.343	-58.498	103.807	1.00	37.93	A
C											

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ATOM    899  C   THR A 235     235.689 -61.252 104.654  1.00 47.59      A
C
ATOM    900  O   THR A 235     236.169 -61.504 103.551  1.00 49.69      A
O
ATOM    901  N   TYR A 236     236.310 -61.521 105.813  1.00 47.35      A
N
ATOM    902  CA  TYR A 236     237.613 -62.189 105.850  1.00 46.90      A
C
ATOM    903  CB  TYR A 236     238.206 -62.221 107.255  1.00 42.67      A
C
ATOM    904  CG  TYR A 236     239.024 -61.003 107.621  1.00 45.24      A
C
ATOM    905  CD1 TYR A 236     239.154 -59.930 106.767  1.00 40.32      A
C
ATOM    906  CE1 TYR A 236     239.909 -58.819 107.134  1.00 51.10      A
C
ATOM    907  CD2 TYR A 236     239.667 -60.929 108.847  1.00 46.47      A
C
ATOM    908  CE2 TYR A 236     240.430 -59.808 109.228  1.00 52.60      A
C
ATOM    909  CZ  TYR A 236     240.542 -58.764 108.367  1.00 49.08      A
C
ATOM    910  OH  TYR A 236     241.265 -57.653 108.719  1.00 58.26      A
O
ATOM    911  C   TYR A 236     237.496 -63.604 105.334  1.00 47.98      A
C
ATOM    912  O   TYR A 236     238.469 -64.148 104.832  1.00 58.71      A
O
ATOM    913  N   ILE A 237     236.296 -64.177 105.416  1.00 50.41      A
N
ATOM    914  CA  ILE A 237     236.032 -65.540 104.944  1.00 46.45      A
C
ATOM    915  CB  ILE A 237     234.816 -66.156 105.635  1.00 45.13      A
C
ATOM    916  CG2 ILE A 237     234.357 -67.442 104.903  1.00 42.23      A
C
ATOM    917  CG1 ILE A 237     235.157 -66.440 107.101  1.00 42.93      A
C
ATOM    918  CD1 ILE A 237     236.253 -67.436 107.317  1.00 39.73      A
C
ATOM    919  C   ILE A 237     235.798 -65.597 103.462  1.00 51.53      A
C
ATOM    920  O   ILE A 237     236.213 -66.548 102.822  1.00 55.68      A
O
ATOM    921  N   THR A 238     235.148 -64.571 102.914  1.00 51.45      A
N
ATOM    922  CA  THR A 238     234.858 -64.526 101.471  1.00 44.65      A
C
ATOM    923  CB  THR A 238     233.929 -63.346 101.106  1.00 44.82      A
C
ATOM    924  OG1 THR A 238     232.653 -63.512 101.719  1.00 43.65      A
O
ATOM    925  CG2 THR A 238     233.701 -63.294  99.660  1.00 44.50      A
C
ATOM    926  C   THR A 238     236.166 -64.350 100.706  1.00 47.18      A
C
ATOM    927  O   THR A 238     236.467 -65.090  99.782  1.00 48.37      A
O
ATOM    928  N   GLU A 239     236.956 -63.367 101.116  1.00 49.98      A
N
ATOM    929  CA  GLU A 239     238.239 -63.082 100.473  1.00 52.23      A
C
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ATOM	930	CB	GLU	A	239	238.937	-61.932	101.203	1.00	54.22	A
C											
ATOM	931	CG	GLU	A	239	238.139	-60.624	101.260	1.00	55.95	A
C											
ATOM	932	CD	GLU	A	239	238.811	-59.573	102.137	1.00	58.38	A
C											
ATOM	933	OE1	GLU	A	239	239.056	-59.843	103.333	1.00	65.65	A
O											
ATOM	934	OE2	GLU	A	239	239.099	-58.468	101.634	1.00	60.73	A
O											
ATOM	935	C	GLU	A	239	239.109	-64.330	100.496	1.00	50.02	A
C											
ATOM	936	O	GLU	A	239	239.851	-64.616	99.561	1.00	55.72	A
O											
ATOM	937	N	LEU	A	240	238.978	-65.104	101.557	1.00	49.14	A
N											
ATOM	938	CA	LEU	A	240	239.768	-66.305	101.702	1.00	48.27	A
C											
ATOM	939	CB	LEU	A	240	239.776	-66.717	103.173	1.00	46.82	A
C											
ATOM	940	CG	LEU	A	240	240.917	-67.581	103.679	1.00	45.79	A
C											
ATOM	941	CD1	LEU	A	240	242.225	-67.030	103.195	1.00	50.28	A
C											
ATOM	942	CD2	LEU	A	240	240.885	-67.603	105.172	1.00	53.83	A
C											
ATOM	943	C	LEU	A	240	239.209	-67.420	100.833	1.00	49.65	A
C											
ATOM	944	O	LEU	A	240	239.960	-68.170	100.210	1.00	53.66	A
O											
ATOM	945	N	ALA	A	241	237.883	-67.519	100.778	1.00	45.02	A
N											
ATOM	946	CA	ALA	A	241	237.222	-68.549	99.965	1.00	50.04	A
C											
ATOM	947	CB	ALA	A	241	235.724	-68.611	100.256	1.00	39.53	A
C											
ATOM	948	C	ALA	A	241	237.447	-68.278	98.481	1.00	47.71	A
C											
ATOM	949	O	ALA	A	241	237.495	-69.203	97.682	1.00	54.94	A
O											
ATOM	950	N	ASN	A	242	237.585	-67.012	98.114	1.00	49.50	A
N											
ATOM	951	CA	ASN	A	242	237.839	-66.637	96.729	1.00	51.78	A
C											
ATOM	952	CB	ASN	A	242	237.688	-65.134	96.554	1.00	45.48	A
C											
ATOM	953	CG	ASN	A	242	236.231	-64.680	96.592	1.00	51.39	A
C											
ATOM	954	OD1	ASN	A	242	235.972	-63.489	96.769	1.00	50.23	A
O											
ATOM	955	ND2	ASN	A	242	235.276	-65.620	96.412	1.00	43.58	A
N											
ATOM	956	C	ASN	A	242	239.241	-67.046	96.330	1.00	50.85	A
C											
ATOM	957	O	ASN	A	242	239.419	-67.736	95.323	1.00	53.87	A
O											
ATOM	958	N	ALA	A	243	240.230	-66.625	97.119	1.00	48.27	A
N											
ATOM	959	CA	ALA	A	243	241.629	-66.970	96.861	1.00	42.21	A
C											
ATOM	960	CB	ALA	A	243	242.534	-66.345	97.913	1.00	45.13	A
C											

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ATOM    961  C   ALA A 243     241.816 -68.473  96.880  1.00 43.95      A
C
ATOM    962  O   ALA A 243     242.498 -69.016  96.026  1.00 42.43      A
O
ATOM    963  N   LEU A 244     241.219 -69.152  97.858  1.00 40.59      A
N
ATOM    964  CA  LEU A 244     241.366 -70.606  97.945  1.00 48.68      A
C
ATOM    965  CB  LEU A 244     240.689 -71.141  99.204  1.00 42.37      A
C
ATOM    966  CG  LEU A 244     241.465 -70.944 100.495  1.00 39.60      A
C
ATOM    967  CD1 LEU A 244     240.751 -71.763 101.602  1.00 37.99      A
C
ATOM    968  CD2 LEU A 244     242.889 -71.432 100.340  1.00 35.22      A
C
ATOM    969  C   LEU A 244     240.779 -71.311  96.702  1.00 56.87      A
C
ATOM    970  O   LEU A 244     241.327 -72.330  96.220  1.00 60.52      A
O
ATOM    971  N   SER A 245     239.662 -70.777  96.200  1.00 61.51      A
N
ATOM    972  CA  SER A 245     239.010 -71.317  95.018  1.00 61.35      A
C
ATOM    973  CB  SER A 245     237.785 -70.501  94.692  1.00 64.64      A
C
ATOM    974  OG  SER A 245     237.339 -70.779  93.390  1.00 71.14      A
O
ATOM    975  C   SER A 245     239.981 -71.242  93.855  1.00 63.54      A
C
ATOM    976  O   SER A 245     240.179 -72.233  93.134  1.00 63.37      A
O
ATOM    977  N   TYR A 246     240.581 -70.063  93.679  1.00 58.29      A
N
ATOM    978  CA  TYR A 246     241.571 -69.855  92.633  1.00 57.08      A
C
ATOM    979  CB  TYR A 246     242.123 -68.455  92.719  1.00 51.38      A
C
ATOM    980  CG  TYR A 246     243.247 -68.195  91.754  1.00 55.36      A
C
ATOM    981  CD1 TYR A 246     242.994 -67.652  90.492  1.00 50.94      A
C
ATOM    982  CE1 TYR A 246     244.042 -67.382  89.609  1.00 55.86      A
C
ATOM    983  CD2 TYR A 246     244.584 -68.473  92.111  1.00 54.39      A
C
ATOM    984  CE2 TYR A 246     245.650 -68.213  91.234  1.00 55.81      A
C
ATOM    985  CZ  TYR A 246     245.372 -67.665  89.982  1.00 55.07      A
C
ATOM    986  OH  TYR A 246     246.409 -67.409  89.112  1.00 55.05      A
O
ATOM    987  C   TYR A 246     242.732 -70.852  92.733  1.00 57.54      A
C
ATOM    988  O   TYR A 246     243.234 -71.322  91.718  1.00 64.40      A
O
ATOM    989  N   CYS A 247     243.150 -71.180  93.951  1.00 56.76      A
N
ATOM    990  CA  CYS A 247     244.245 -72.120  94.148  1.00 57.81      A
C
ATOM    991  CB  CYS A 247     244.779 -72.066  95.599  1.00 52.55      A
C
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ATOM    992  SG  CYS A 247     245.687 -70.569  96.004  1.00 57.32      A
S
ATOM    993  C   CYS A 247     243.813 -73.538  93.837  1.00 59.03      A
C
ATOM    994  O   CYS A 247     244.535 -74.272  93.143  1.00 61.55      A
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ATOM    995  N   HIS A 248     242.659 -73.930  94.374  1.00 60.08      A
N
ATOM    996  CA  HIS A 248     242.151 -75.291  94.156  1.00 58.63      A
C
ATOM    997  CB  HIS A 248     240.916 -75.540  95.036  1.00 57.40      A
C
ATOM    998  CG  HIS A 248     241.217 -75.606  96.496  1.00 54.60      A
C
ATOM    999  CD2 HIS A 248     242.393 -75.694  97.160  1.00 54.55      A
C
ATOM   1000  ND1 HIS A 248     240.231 -75.623  97.459  1.00 54.23      A
N
ATOM   1001  CE1 HIS A 248     240.789 -75.721  98.654  1.00 51.97      A
C
ATOM   1002  NE2 HIS A 248     242.099 -75.765  98.501  1.00 50.58      A
N
ATOM   1003  C   HIS A 248     241.806 -75.535  92.668  1.00 58.67      A
C
ATOM   1004  O   HIS A 248     241.857 -76.667  92.171  1.00 50.45      A
O
ATOM   1005  N   SER A 249     241.459 -74.464  91.959  1.00 53.97      A
N
ATOM   1006  CA  SER A 249     241.133 -74.589  90.550  1.00 58.32      A
C
ATOM   1007  CB  SER A 249     240.647 -73.248  89.991  1.00 55.40      A
C
ATOM   1008  OG  SER A 249     241.757 -72.480  89.526  1.00 54.94      A
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ATOM   1009  C   SER A 249     242.407 -75.020  89.798  1.00 58.15      A
C
ATOM   1010  O   SER A 249     242.326 -75.573  88.707  1.00 70.94      A
O
ATOM   1011  N   LYS A 250     243.574 -74.746  90.370  1.00 51.49      A
N
ATOM   1012  CA  LYS A 250     244.820 -75.119  89.753  1.00 46.67      A
C
ATOM   1013  CB  LYS A 250     245.818 -73.947  89.805  1.00 31.37      A
C
ATOM   1014  C   LYS A 250     245.364 -76.343  90.494  1.00 50.71      A
C
ATOM   1015  O   LYS A 250     246.506 -76.755  90.233  1.00 60.01      A
O
ATOM   1016  N   ARG A 251     244.553 -76.931  91.389  1.00 52.78      A
N
ATOM   1017  CA  ARG A 251     244.965 -78.113  92.167  1.00 55.47      A
C
ATOM   1018  CB  ARG A 251     245.383 -79.258  91.244  1.00 58.86      A
C
ATOM   1019  CG  ARG A 251     244.211 -79.957  90.536  1.00 62.01      A
C
ATOM   1020  CD  ARG A 251     244.126 -81.392  90.989  1.00 65.71      A
C
ATOM   1021  NE  ARG A 251     242.807 -81.741  91.512  1.00 68.34      A
N
ATOM   1022  CZ  ARG A 251     242.484 -82.945  92.002  1.00 72.31      A
C
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ATOM 1023 NH1 ARG A 251 243.384 -83.929 92.045 1.00 72.96 A
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ATOM 1024 NH2 ARG A 251 241.252 -83.178 92.445 1.00 71.74 A
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ATOM 1025 C ARG A 251 246.099 -77.840 93.137 1.00 53.93 A
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ATOM 1026 O ARG A 251 247.007 -78.666 93.285 1.00 57.77 A
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ATOM 1027 N VAL A 252 246.043 -76.686 93.799 1.00 56.22 A
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ATOM 1028 CA VAL A 252 247.072 -76.314 94.774 1.00 53.20 A
C
ATOM 1029 CB VAL A 252 247.721 -74.966 94.401 1.00 50.06 A
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ATOM 1030 CG1 VAL A 252 248.682 -74.549 95.463 1.00 49.54 A
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ATOM 1031 CG2 VAL A 252 248.418 -75.083 93.080 1.00 48.46 A
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ATOM 1032 C VAL A 252 246.492 -76.207 96.196 1.00 54.67 A
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ATOM 1033 O VAL A 252 245.536 -75.465 96.426 1.00 56.55 A
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ATOM 1034 N ILE A 253 247.074 -76.956 97.130 1.00 52.34 A
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ATOM 1035 CA ILE A 253 246.641 -76.948 98.498 1.00 42.71 A
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ATOM 1036 CB ILE A 253 246.696 -78.341 99.103 1.00 38.24 A
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ATOM 1037 CG2 ILE A 253 245.676 -78.449 100.219 1.00 44.12 A
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ATOM 1038 CG1 ILE A 253 246.279 -79.380 98.083 1.00 35.92 A
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ATOM 1039 CD1 ILE A 253 246.298 -80.813 98.644 1.00 42.55 A
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ATOM 1040 C ILE A 253 247.600 -76.096 99.279 1.00 48.08 A
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ATOM 1041 O ILE A 253 248.808 -76.288 99.163 1.00 60.87 A
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ATOM 1042 N HIS A 254 247.084 -75.165 100.086 1.00 50.60 A
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ATOM 1043 CA HIS A 254 247.955 -74.319 100.906 1.00 45.11 A
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ATOM 1044 CB HIS A 254 247.187 -73.086 101.374 1.00 43.92 A
C
ATOM 1045 CG HIS A 254 248.071 -72.014 101.916 1.00 44.85 A
C
ATOM 1046 CD2 HIS A 254 248.486 -70.854 101.360 1.00 39.20 A
C
ATOM 1047 ND1 HIS A 254 248.670 -72.089 103.158 1.00 39.59 A
N
ATOM 1048 CE1 HIS A 254 249.414 -71.014 103.339 1.00 37.61 A
C
ATOM 1049 NE2 HIS A 254 249.318 -70.250 102.265 1.00 38.54 A
N
ATOM 1050 C HIS A 254 248.490 -75.117 102.103 1.00 44.15 A
C
ATOM 1051 O HIS A 254 249.681 -75.123 102.372 1.00 48.22 A
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ATOM 1052 N ARG A 255 247.587 -75.802 102.793 1.00 42.94 A
N
ATOM 1053 CA ARG A 255 247.899 -76.642 103.946 1.00 38.93 A
C

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ATOM   1054  CB  ARG A 255     248.829 -77.796 103.512  1.00 44.03      A
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ATOM   1267  CA  SER A 283     249.163 -85.680  98.758  1.00 59.53      A
C
ATOM   1268  CB  SER A 283     250.127 -84.498  98.799  1.00 55.46      A
C
ATOM   1269  OG  SER A 283     250.750 -84.456 100.075  1.00 55.84      A
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ATOM   1270  C   SER A 283     249.259 -86.394 100.033  1.00 55.99      A
C
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ATOM   1271  O   SER A 283     248.283 -86.609 100.713  1.00 69.93      A
O
ATOM   1272  N   SER A 284     250.462 -86.835 100.323  1.00 60.56      A
N
ATOM   1273  CA  SER A 284     250.699 -87.467 101.588  1.00 63.49      A
C
ATOM   1274  CB  SER A 284     251.416 -88.808 101.438  1.00 63.76      A
C
ATOM   1275  OG  SER A 284     252.588 -88.697 100.633  1.00 77.24      A
O
ATOM   1276  C   SER A 284     251.609 -86.432 102.280  1.00 63.54      A
C
ATOM   1277  O   SER A 284     251.934 -85.336 101.744  1.00 57.98      A
O
ATOM   1278  N   ARG A 285     251.999 -86.775 103.492  1.00 64.16      A
N
ATOM   1279  CA  ARG A 285     252.823 -85.889 104.282  1.00 67.66      A
C
ATOM   1280  CB  ARG A 285     252.738 -86.301 105.734  1.00 62.91      A
C
ATOM   1281  C   ARG A 285     254.278 -85.923 103.806  1.00 68.61      A
C
ATOM   1282  O   ARG A 285     254.612 -86.645 102.888  1.00 72.84      A
O
ATOM   1283  N   ARG A 286     255.135 -85.146 104.466  1.00 71.24      A
N
ATOM   1284  CA  ARG A 286     256.561 -85.059 104.163  1.00 75.06      A
C
ATOM   1285  CB  ARG A 286     256.943 -83.563 104.008  1.00 73.44      A
C
ATOM   1286  CG  ARG A 286     255.881 -82.698 103.382  1.00 71.75      A
C
ATOM   1287  CD  ARG A 286     255.139 -83.449 102.361  1.00 72.37      A
C
ATOM   1288  NE  ARG A 286     255.481 -82.999 101.030  1.00 72.92      A
N
ATOM   1289  CZ  ARG A 286     254.690 -83.207  99.989  1.00 77.01      A
C
ATOM   1290  NH1 ARG A 286     253.537 -83.858 100.174  1.00 80.80      A
N
ATOM   1291  NH2 ARG A 286     255.024 -82.753  98.778  1.00 73.00      A
N
ATOM   1292  C   ARG A 286     257.251 -85.649 105.339  1.00 79.18      A
C
ATOM   1293  O   ARG A 286     258.525 -85.258 105.556  1.00 80.60      A
O
ATOM   1294  N   TPO A 287     256.458 -86.471 106.097  1.00 82.59      A
N
ATOM   1295  CA  TPO A 287     256.848 -87.091 107.376  1.00 81.36      A
C
ATOM   1296  CB  TPO A 287     258.340 -87.583 107.506  1.00 85.77      A
C
ATOM   1297  CG2 TPO A 287     258.788 -88.436 108.791  1.00 78.62      A
C
ATOM   1298  OG1 TPO A 287     259.242 -87.965 106.406  1.00 96.25      A
O
ATOM   1299  P   TPO A 287     259.671 -89.537 105.840  1.00 94.10      A
P
ATOM   1300  O1P TPO A 287     261.195 -89.889 106.372  1.00105.80      A
O
ATOM   1301  O2P TPO A 287     259.793 -89.485 104.142  1.00103.14      A
O
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ATOM   1302  O3P TPO A 287     258.773 -90.552 106.786  1.00103.19      A
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ATOM   1303  C   TPO A 287     257.020 -86.093 108.560  1.00 84.40      A
C
ATOM   1304  O   TPO A 287     256.708 -86.453 109.760  1.00 82.15      A
O
ATOM   1305  N   TPO A 288     257.164 -84.776 108.357  1.00 86.52      A
N
ATOM   1306  CA  TPO A 288     257.256 -84.113 109.592  1.00 85.55      A
C
ATOM   1307  CB  TPO A 288     258.562 -83.387 109.678  1.00 87.59      A
C
ATOM   1308  CG2 TPO A 288     259.265 -83.063 111.066  1.00 82.26      A
C
ATOM   1309  OG1 TPO A 288     259.687 -83.759 108.739  1.00 93.55      A
O
ATOM   1310  P   TPO A 288     261.048 -84.822 108.978  1.00 87.77      A
P
ATOM   1311  O1P TPO A 288     262.388 -83.892 109.216  1.00 91.79      A
O
ATOM   1312  O2P TPO A 288     261.352 -85.656 107.542  1.00 93.35      A
O
ATOM   1313  O3P TPO A 288     260.797 -85.456 110.481  1.00 95.16      A
O
ATOM   1314  C   TPO A 288     256.287 -82.985 109.892  1.00 89.28      A
C
ATOM   1315  O   TPO A 288     255.311 -82.594 109.048  1.00 86.14      A
O
ATOM   1316  N   LEU A 289     256.536 -82.411 111.055  1.00 87.01      A
N
ATOM   1317  CA  LEU A 289     255.511 -81.523 111.435  1.00 88.25      A
C
ATOM   1318  CB  LEU A 289     254.346 -82.345 111.883  1.00 78.91      A
C
ATOM   1319  C   LEU A 289     255.852 -80.565 112.436  1.00 87.34      A
C
ATOM   1320  O   LEU A 289     256.026 -80.894 113.634  1.00 90.27      A
O
ATOM   1321  N   CYS A 290     256.101 -79.389 111.914  1.00 89.51      A
N
ATOM   1322  CA  CYS A 290     256.347 -78.354 112.824  1.00 89.73      A
C
ATOM   1323  CB  CYS A 290     257.299 -77.405 112.324  1.00 80.05      A
C
ATOM   1324  C   CYS A 290     254.931 -77.891 112.490  1.00 90.22      A
C
ATOM   1325  O   CYS A 290     254.405 -77.933 111.292  1.00 91.11      A
O
ATOM   1326  N   GLY A 291     254.262 -77.496 113.541  1.00 90.88      A
N
ATOM   1327  CA  GLY A 291     252.946 -77.026 113.294  1.00 84.36      A
C
ATOM   1328  C   GLY A 291     252.214 -77.175 114.559  1.00 80.67      A
C
ATOM   1329  O   GLY A 291     252.395 -78.093 115.381  1.00 72.19      A
O
ATOM   1330  N   THR A 292     251.411 -76.152 114.668  1.00 72.87      A
N
ATOM   1331  CA  THR A 292     250.543 -75.923 115.732  1.00 68.66      A
C
ATOM   1332  CB  THR A 292     250.229 -74.450 115.788  1.00 64.26      A
C
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ATOM   1333  OG1 THR A 292     249.385 -74.238 116.907  1.00 62.83      A
O
ATOM   1334  CG2 THR A 292     249.511 -73.967 114.478  1.00 66.76      A
C
ATOM   1335  C   THR A 292     249.401 -76.698 115.093  1.00 69.67      A
C
ATOM   1336  O   THR A 292     248.736 -76.230 114.162  1.00 81.32      A
O
ATOM   1337  N   LEU A 293     249.162 -77.905 115.545  1.00 65.76      A
N
ATOM   1338  CA  LEU A 293     248.076 -78.633 114.929  1.00 57.85      A
C
ATOM   1339  CB  LEU A 293     247.775 -79.863 115.741  1.00 58.26      A
C
ATOM   1340  CG  LEU A 293     249.007 -80.649 116.175  1.00 59.75      A
C
ATOM   1341  CD1 LEU A 293     248.607 -81.606 117.246  1.00 56.85      A
C
ATOM   1342  CD2 LEU A 293     249.618 -81.397 114.982  1.00 55.33      A
C
ATOM   1343  C   LEU A 293     246.812 -77.819 114.737  1.00 54.37      A
C
ATOM   1344  O   LEU A 293     246.215 -77.930 113.686  1.00 59.11      A
O
ATOM   1345  N   ASP A 294     246.467 -76.947 115.687  1.00 45.72      A
N
ATOM   1346  CA  ASP A 294     245.241 -76.166 115.622  1.00 46.04      A
C
ATOM   1347  CB  ASP A 294     245.471 -74.762 116.195  1.00 47.18      A
C
ATOM   1348  CG  ASP A 294     245.754 -74.782 117.713  1.00 53.87      A
C
ATOM   1349  OD1 ASP A 294     244.938 -75.399 118.452  1.00 53.07      A
O
ATOM   1350  OD2 ASP A 294     246.772 -74.166 118.153  1.00 44.18      A
O
ATOM   1351  C   ASP A 294     244.490 -76.064 114.323  1.00 42.63      A
C
ATOM   1352  O   ASP A 294     243.322 -76.434 114.275  1.00 40.46      A
O
ATOM   1353  N   TYR A 295     245.168 -75.589 113.280  1.00 41.51      A
N
ATOM   1354  CA  TYR A 295     244.534 -75.404 111.983  1.00 42.29      A
C
ATOM   1355  CB  TYR A 295     245.046 -74.116 111.335  1.00 42.13      A
C
ATOM   1356  CG  TYR A 295     245.120 -72.945 112.263  1.00 41.89      A
C
ATOM   1357  CD1 TYR A 295     246.211 -72.793 113.099  1.00 47.14      A
C
ATOM   1358  CE1 TYR A 295     246.304 -71.731 113.973  1.00 47.33      A
C
ATOM   1359  CD2 TYR A 295     244.117 -71.995 112.309  1.00 36.13      A
C
ATOM   1360  CE2 TYR A 295     244.212 -70.914 113.162  1.00 43.23      A
C
ATOM   1361  CZ  TYR A 295     245.302 -70.785 113.996  1.00 47.19      A
C
ATOM   1362  OH  TYR A 295     245.414 -69.690 114.838  1.00 57.32      A
O
ATOM   1363  C   TYR A 295     244.655 -76.563 110.985  1.00 41.49      A
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ATOM   1364  O   TYR A 295     244.224 -76.467 109.822  1.00 43.26      A
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ATOM   1365  N   LEU A 296     245.228 -77.668 111.448  1.00 39.99      A
N
ATOM   1366  CA  LEU A 296     245.411 -78.868 110.607  1.00 51.39      A
C
ATOM   1367  CB  LEU A 296     246.671 -79.611 111.016  1.00 53.81      A
C
ATOM   1368  CG  LEU A 296     248.033 -78.987 110.652  1.00 57.41      A
C
ATOM   1369  CD1 LEU A 296     249.165 -79.934 111.025  1.00 51.84      A
C
ATOM   1370  CD2 LEU A 296     248.040 -78.694 109.161  1.00 50.59      A
C
ATOM   1371  C   LEU A 296     244.205 -79.803 110.651  1.00 48.90      A
C
ATOM   1372  O   LEU A 296     243.511 -79.890 111.645  1.00 60.00      A
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ATOM   1373  N   PRO A 297     243.914 -80.480 109.550  1.00 49.64      A
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ATOM   1374  CD  PRO A 297     244.428 -80.152 108.220  1.00 48.93      A
C
ATOM   1375  CA  PRO A 297     242.782 -81.390 109.447  1.00 53.31      A
C
ATOM   1376  CB  PRO A 297     242.450 -81.327 107.951  1.00 50.04      A
C
ATOM   1377  CG  PRO A 297     243.782 -81.194 107.367  1.00 48.93      A
C
ATOM   1378  C   PRO A 297     243.137 -82.762 109.966  1.00 57.23      A
C
ATOM   1379  O   PRO A 297     244.303 -83.109 110.051  1.00 56.18      A
O
ATOM   1380  N   PRO A 298     242.135 -83.562 110.334  1.00 59.72      A
N
ATOM   1381  CD  PRO A 298     240.704 -83.237 110.308  1.00 64.33      A
C
ATOM   1382  CA  PRO A 298     242.340 -84.917 110.853  1.00 62.61      A
C
ATOM   1383  CB  PRO A 298     240.929 -85.463 110.920  1.00 65.22      A
C
ATOM   1384  CG  PRO A 298     240.143 -84.267 111.288  1.00 64.88      A
C
ATOM   1385  C   PRO A 298     243.245 -85.779 109.963  1.00 64.63      A
C
ATOM   1386  O   PRO A 298     244.184 -86.426 110.459  1.00 56.23      A
O
ATOM   1387  N   GLU A 299     242.975 -85.781 108.656  1.00 60.03      A
N
ATOM   1388  CA  GLU A 299     243.778 -86.574 107.711  1.00 58.56      A
C
ATOM   1389  CB  GLU A 299     243.303 -86.339 106.265  1.00 57.01      A
C
ATOM   1390  CG  GLU A 299     243.028 -84.864 105.914  1.00 52.94      A
C
ATOM   1391  CD  GLU A 299     241.596 -84.474 106.109  1.00 48.80      A
C
ATOM   1392  OE1 GLU A 299     241.003 -84.897 107.126  1.00 47.74      A
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ATOM   1393  OE2 GLU A 299     241.075 -83.733 105.248  1.00 48.97      A
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ATOM   1394  C   GLU A 299     245.279 -86.287 107.819  1.00 62.41      A
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ATOM   1395  O   GLU A 299     246.094 -87.208 108.002  1.00 64.05      A
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ATOM   1396  N   MET A 300     245.648 -85.014 107.709  1.00 63.79      A
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ATOM   1397  CA  MET A 300     247.051 -84.637 107.816  1.00 63.71      A
C
ATOM   1398  CB  MET A 300     247.225 -83.145 107.597  1.00 67.63      A
C
ATOM   1399  CG  MET A 300     247.374 -82.763 106.145  1.00 66.70      A
C
ATOM   1400  SD  MET A 300     248.052 -81.127 106.017  1.00 71.20      A
S
ATOM   1401  CE  MET A 300     249.750 -81.388 106.380  1.00 69.10      A
C
ATOM   1402  C   MET A 300     247.661 -85.000 109.174  1.00 66.02      A
C
ATOM   1403  O   MET A 300     248.702 -85.664 109.256  1.00 70.05      A
O
ATOM   1404  N   ILE A 301     247.025 -84.550 110.244  1.00 67.53      A
N
ATOM   1405  CA  ILE A 301     247.504 -84.829 111.596  1.00 68.63      A
C
ATOM   1406  CB  ILE A 301     246.490 -84.278 112.606  1.00 67.77      A
C
ATOM   1407  CG2 ILE A 301     246.782 -84.750 113.995  1.00 61.97      A
C
ATOM   1408  CG1 ILE A 301     246.505 -82.750 112.495  1.00 67.98      A
C
ATOM   1409  CD1 ILE A 301     245.392 -82.041 113.240  1.00 76.63      A
C
ATOM   1410  C   ILE A 301     247.769 -86.319 111.812  1.00 73.57      A
C
ATOM   1411  O   ILE A 301     248.662 -86.676 112.588  1.00 78.37      A
O
ATOM   1412  N   GLU A 302     247.034 -87.184 111.092  1.00 75.18      A
N
ATOM   1413  CA  GLU A 302     247.212 -88.639 111.215  1.00 74.73      A
C
ATOM   1414  CB  GLU A 302     245.845 -89.306 111.428  1.00 70.49      A
C
ATOM   1415  CG  GLU A 302     245.378 -89.254 112.936  1.00 78.38      A
C
ATOM   1416  CD  GLU A 302     243.861 -89.396 113.127  1.00 79.55      A
C
ATOM   1417  OE1 GLU A 302     243.188 -90.062 112.281  1.00 80.35      A
O
ATOM   1418  OE2 GLU A 302     243.360 -88.836 114.140  1.00 87.62      A
O
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C
ATOM   1420  O   GLU A 302     248.411 -90.458 110.160  1.00 81.76      A
O
ATOM   1421  N   GLY A 303     248.339 -88.531 109.006  1.00 78.40      A
N
ATOM   1422  CA  GLY A 303     249.160 -89.053 107.912  1.00 72.91      A
C
ATOM   1423  C   GLY A 303     248.566 -89.374 106.552  1.00 72.79      A
C
ATOM   1424  O   GLY A 303     249.237 -89.368 105.513  1.00 76.85      A
O
ATOM   1425  N   ARG A 304     247.286 -89.679 106.549  1.00 67.34      A
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ATOM   1426  CA  ARG A 304     246.623 -90.043 105.300  1.00 63.57      A
C
ATOM   1427  CB  ARG A 304     245.098 -90.120 105.461  1.00 62.11      A
C
ATOM   1428  CG  ARG A 304     244.623 -91.200 106.414  1.00 63.49      A
C
ATOM   1429  CD  ARG A 304     243.198 -90.950 106.857  1.00 70.18      A
C
ATOM   1430  NE  ARG A 304     243.087 -89.787 107.759  1.00 79.24      A
N
ATOM   1431  CZ  ARG A 304     242.896 -89.857 109.080  1.00 78.33      A
C
ATOM   1432  NH1 ARG A 304     242.788 -91.031 109.665  1.00 78.68      A
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ATOM   1433  NH2 ARG A 304     242.819 -88.757 109.821  1.00 83.87      A
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ATOM   1434  C   ARG A 304     246.882 -89.200 104.087  1.00 60.49      A
C
ATOM   1435  O   ARG A 304     247.550 -88.195 104.122  1.00 65.51      A
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N
ATOM   1437  CA  MET A 305     246.335 -89.084 101.698  1.00 65.46      A
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ATOM   1438  CB  MET A 305     246.041 -90.197 100.663  1.00 63.39      A
C
ATOM   1439  C   MET A 305     245.233 -88.042 101.699  1.00 69.37      A
C
ATOM   1440  O   MET A 305     244.036 -88.349 101.691  1.00 78.96      A
O
ATOM   1441  N   HIS A 306     245.671 -86.802 101.710  1.00 69.56      A
N
ATOM   1442  CA  HIS A 306     244.790 -85.674 101.706  1.00 64.25      A
C
ATOM   1443  CB  HIS A 306     245.247 -84.657 102.735  1.00 64.47      A
C
ATOM   1444  CG  HIS A 306     246.674 -84.276 102.611  1.00 58.72      A
C
ATOM   1445  CD2 HIS A 306     247.253 -83.167 102.099  1.00 56.35      A
C
ATOM   1446  ND1 HIS A 306     247.691 -85.072 103.092  1.00 58.38      A
N
ATOM   1447  CE1 HIS A 306     248.841 -84.461 102.883  1.00 55.77      A
C
ATOM   1448  NE2 HIS A 306     248.602 -83.307 102.284  1.00 54.24      A
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ATOM   1449  C   HIS A 306     244.657 -85.001 100.363  1.00 64.13      A
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ATOM   1452  CA  ASP A 307     243.316 -83.353  99.117  1.00 67.53      A
C
ATOM   1453  CB  ASP A 307     241.988 -83.886  98.618  1.00 76.36      A
C
ATOM   1454  CG  ASP A 307     241.022 -84.130  99.789  1.00 82.91      A
C
ATOM   1455  OD1 ASP A 307     240.938 -83.232 100.665  1.00 87.78      A
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ATOM   1456  OD2 ASP A 307     240.376 -85.208  99.863  1.00 84.54      A
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ATOM   1457  C   ASP A 307     243.130 -81.873  99.495  1.00 62.06      A
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ATOM   1458  O   ASP A 307     243.430 -81.435 100.603  1.00 62.07      A
O
ATOM   1459  N   GLU A 308     242.537 -81.150  98.566  1.00 56.29      A
N
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C
ATOM   1461  CB  GLU A 308     241.830 -79.236  97.325  1.00 58.22      A
C
ATOM   1462  CG  GLU A 308     241.947 -80.428  96.353  1.00 63.76      A
C
ATOM   1463  CD  GLU A 308     241.729 -80.087  94.898  1.00 66.66      A
C
ATOM   1464  OE1 GLU A 308     242.570 -79.367  94.305  1.00 69.11      A
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ATOM   1465  OE2 GLU A 308     240.722 -80.565  94.330  1.00 69.49      A
O
ATOM   1466  C   GLU A 308     241.201 -79.444  99.802  1.00 56.96      A
C
ATOM   1467  O   GLU A 308     241.003 -78.286 100.226  1.00 57.79      A
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ATOM   1468  N   LYS A 309     240.558 -80.495 100.296  1.00 54.61      A
N
ATOM   1469  CA  LYS A 309     239.526 -80.332 101.317  1.00 54.70      A
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ATOM   1470  CB  LYS A 309     238.697 -81.615 101.449  1.00 46.40      A
C
ATOM   1471  CG  LYS A 309     237.740 -81.859 100.300  1.00 53.44      A
C
ATOM   1472  CD  LYS A 309     236.674 -80.778 100.253  1.00 58.61      A
C
ATOM   1473  CE  LYS A 309     235.600 -81.071  99.214  1.00 60.43      A
C
ATOM   1474  NZ  LYS A 309     234.524 -80.026  99.209  1.00 60.76      A
N
ATOM   1475  C   LYS A 309     240.111 -79.967 102.668  1.00 54.64      A
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ATOM   1476  O   LYS A 309     239.366 -79.724 103.618  1.00 66.35      A
O
ATOM   1477  N   VAL A 310     241.439 -79.941 102.770  1.00 57.91      A
N
ATOM   1478  CA  VAL A 310     242.086 -79.593 104.039  1.00 53.66      A
C
ATOM   1479  CB  VAL A 310     243.573 -79.974 104.058  1.00 52.18      A
C
ATOM   1480  CG1 VAL A 310     243.749 -81.375 103.528  1.00 54.98      A
C
ATOM   1481  CG2 VAL A 310     244.347 -79.010 103.252  1.00 55.72      A
C
ATOM   1482  C   VAL A 310     241.957 -78.091 104.263  1.00 53.64      A
C
ATOM   1483  O   VAL A 310     241.771 -77.638 105.404  1.00 47.54      A
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ATOM   1484  N   ASP A 311     242.008 -77.332 103.168  1.00 50.01      A
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ATOM   1485  CA  ASP A 311     241.881 -75.889 103.255  1.00 57.45      A
C
ATOM   1486  CB  ASP A 311     242.275 -75.232 101.925  1.00 56.10      A
C
ATOM   1487  CG  ASP A 311     243.756 -75.367 101.624  1.00 55.84      A
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ATOM   1491  O   ASP A 311     240.258 -74.365 104.208  1.00 69.75      A
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ATOM   1495  CG  LEU A 312     236.719 -76.481 101.746  1.00 45.65      A
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ATOM   1496  CD1 LEU A 312     236.262 -77.698 100.966  1.00 57.08      A
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ATOM   1497  CD2 LEU A 312     235.607 -75.431 101.878  1.00 42.14      A
C
ATOM   1498  C   LEU A 312     238.066 -76.204 105.309  1.00 42.72      A
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C
ATOM   1503  CG  TRP A 313     239.903 -78.960 108.973  1.00 37.21      A
C
ATOM   1504  CD2 TRP A 313     239.169 -79.815 109.859  1.00 38.09      A
C
ATOM   1505  CE2 TRP A 313     239.786 -79.742 111.133  1.00 40.55      A
C
ATOM   1506  CE3 TRP A 313     238.050 -80.627 109.706  1.00 42.38      A
C
ATOM   1507  CD1 TRP A 313     240.895 -78.418 109.716  1.00 40.67      A
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ATOM   1508  NE1 TRP A 313     240.843 -78.885 111.022  1.00 36.83      A
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ATOM   1509  CZ2 TRP A 313     239.325 -80.470 112.237  1.00 41.12      A
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ATOM   1510  CZ3 TRP A 313     237.591 -81.353 110.817  1.00 40.98      A
C
ATOM   1511  CH2 TRP A 313     238.220 -81.265 112.052  1.00 42.79      A
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ATOM   1512  C   TRP A 313     239.448 -76.259 108.009  1.00 45.03      A
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C
ATOM   1517  OG  SER A 314     243.333 -75.505 107.387  1.00 38.93      A
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ATOM   1518  C   SER A 314     240.338 -73.392 108.062  1.00 39.99      A
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ATOM   1534  CB  VAL A 317     240.378 -73.903 112.348  1.00 39.35      A
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ATOM   1535  CG1 VAL A 317     241.200 -73.322 113.465  1.00 39.07      A
C
ATOM   1536  CG2 VAL A 317     240.268 -75.403 112.500  1.00 36.59      A
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ATOM   1537  C   VAL A 317     239.145 -71.743 112.382  1.00 39.43      A
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ATOM   1538  O   VAL A 317     238.923 -71.092 113.421  1.00 39.97      A
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ATOM   1541  CB  LEU A 318     240.217 -69.443 109.701  1.00 34.72      A
C
ATOM   1542  CG  LEU A 318     241.505 -68.678 109.594  1.00 35.85      A
C
ATOM   1543  CD1 LEU A 318     242.492 -69.129 110.631  1.00 35.87      A
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ATOM   1544  CD2 LEU A 318     242.040 -68.906 108.254  1.00 39.24      A
C
ATOM   1545  C   LEU A 318     238.440 -68.952 111.425  1.00 41.79      A
C
ATOM   1546  O   LEU A 318     238.499 -67.943 112.191  1.00 36.26      A
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ATOM   1547  N   CYS A 319     237.301 -69.398 110.858  1.00 35.62      A
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ATOM   1548  CA  CYS A 319     236.053 -68.700 111.024  1.00 40.61      A
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ATOM   1549  CB  CYS A 319     235.013 -69.338 110.158  1.00 35.35      A
C
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ATOM	1550	SG	CYS	A	319	233.324	-68.489	110.215	1.00	25.40	A
S										
ATOM	1551	C	CYS	A	319	235.640	-68.734	112.482	1.00	35.51	A
C										
ATOM	1552	O	CYS	A	319	235.027	-67.810	112.980	1.00	40.27	A
O										
ATOM	1553	N	TYR	A	320	236.009	-69.795	113.182	1.00	38.46	A
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ATOM	1554	CA	TYR	A	320	235.683	-69.942	114.604	1.00	39.25	A
C										
ATOM	1555	CB	TYR	A	320	235.867	-71.406	115.016	1.00	37.24	A
C										
ATOM	1556	CG	TYR	A	320	235.634	-71.683	116.479	1.00	38.04	A
C										
ATOM	1557	CD1	TYR	A	320	236.573	-71.333	117.438	1.00	34.91	A
C										
ATOM	1558	CE1	TYR	A	320	236.380	-71.640	118.800	1.00	31.79	A
C										
ATOM	1559	CD2	TYR	A	320	234.484	-72.331	116.892	1.00	39.29	A
C										
ATOM	1560	CE2	TYR	A	320	234.248	-72.628	118.233	1.00	35.49	A
C										
ATOM	1561	CZ	TYR	A	320	235.191	-72.289	119.198	1.00	41.97	A
C										
ATOM	1562	OH	TYR	A	320	234.905	-72.575	120.532	1.00	35.00	A
O										
ATOM	1563	C	TYR	A	320	236.613	-69.038	115.435	1.00	43.31	A
C										
ATOM	1564	O	TYR	A	320	236.166	-68.318	116.322	1.00	51.83	A
O										
ATOM	1565	N	GLU	A	321	237.910	-69.073	115.144	1.00	42.04	A
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ATOM	1566	CA	GLU	A	321	238.860	-68.249	115.871	1.00	43.24	A
C										
ATOM	1567	CB	GLU	A	321	240.273	-68.552	115.419	1.00	36.62	A
C										
ATOM	1568	CG	GLU	A	321	241.311	-67.733	116.144	1.00	43.20	A
C										
ATOM	1569	CD	GLU	A	321	242.689	-68.087	115.740	1.00	47.61	A
C										
ATOM	1570	OE1	GLU	A	321	242.845	-69.101	115.003	1.00	49.19	A
O										
ATOM	1571	OE2	GLU	A	321	243.606	-67.350	116.171	1.00	55.54	A
O										
ATOM	1572	C	GLU	A	321	238.569	-66.763	115.714	1.00	42.47	A
C										
ATOM	1573	O	GLU	A	321	238.794	-65.970	116.656	1.00	48.77	A
O										
ATOM	1574	N	PHE	A	322	238.073	-66.377	114.539	1.00	40.79	A
N										
ATOM	1575	CA	PHE	A	322	237.728	-64.970	114.299	1.00	37.96	A
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ATOM	1576	CB	PHE	A	322	237.361	-64.737	112.846	1.00	37.47	A
C										
ATOM	1577	CG	PHE	A	322	238.517	-64.880	111.892	1.00	39.59	A
C										
ATOM	1578	CD1	PHE	A	322	239.839	-64.729	112.338	1.00	34.97	A
C										
ATOM	1579	CD2	PHE	A	322	238.279	-65.133	110.515	1.00	41.97	A
C										
ATOM	1580	CE1	PHE	A	322	240.892	-64.830	111.441	1.00	36.15	A
C										

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ATOM   1581  CE2 PHE A 322     239.342 -65.232 109.605  1.00 35.10      A
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ATOM   1582  CZ  PHE A 322     240.649 -65.081 110.070  1.00 38.47      A
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ATOM   1588  CG  LEU A 323     232.935 -65.689 114.325  1.00 29.77      A
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ATOM   1589  CD1 LEU A 323     231.967 -66.804 113.984  1.00 24.59      A
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ATOM   1590  CD2 LEU A 323     232.306 -64.288 114.046  1.00 30.36      A
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ATOM   1592  O   LEU A 323     234.058 -64.495 118.618  1.00 36.74      A
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ATOM   1595  CB  VAL A 324     235.648 -68.102 119.816  1.00 37.17      A
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ATOM   1596  CG1 VAL A 324     235.879 -68.419 121.294  1.00 34.96      A
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ATOM   1597  CG2 VAL A 324     234.352 -68.697 119.303  1.00 26.08      A
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ATOM   1598  C   VAL A 324     236.903 -66.012 120.154  1.00 35.95      A
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ATOM   1603  O   GLY A 325     241.414 -66.092 120.321  1.00 38.22      A
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ATOM   1604  N   LYS A 326     239.929 -67.663 119.722  1.00 45.05      A
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ATOM   1606  CB  LYS A 326     240.994 -69.180 121.325  1.00 52.62      A
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ATOM   1607  CG  LYS A 326     239.699 -69.600 121.927  1.00 55.78      A
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ATOM   1608  CD  LYS A 326     239.856 -69.912 123.415  1.00 60.70      A
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ATOM   1609  CE  LYS A 326     238.486 -70.233 124.058  1.00 66.17      A
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ATOM   1611  C   LYS A 326     240.419 -69.937 119.005  1.00 46.11      A
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ATOM   1614  CD  PRO A 327     242.773 -70.850 118.901  1.00 43.78      A
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ATOM   1616  CB  PRO A 327     242.331 -72.631 117.446  1.00 38.86      A
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ATOM   1617  CG  PRO A 327     243.349 -71.561 117.738  1.00 42.00      A
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ATOM   1621  CD  PRO A 328     239.083 -73.540 116.278  1.00 35.93      A
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ATOM   1623  CB  PRO A 328     237.340 -74.900 117.106  1.00 40.94      A
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ATOM   1624  CG  PRO A 328     238.298 -74.799 115.948  1.00 38.83      A
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ATOM   1625  C   PRO A 328     238.785 -75.820 118.933  1.00 44.48      A
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ATOM   1629  CB  PHE A 329     241.119 -78.268 118.089  1.00 42.34      A
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ATOM   1630  CG  PHE A 329     240.026 -78.559 117.139  1.00 42.28      A
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ATOM   1631  CD1 PHE A 329     238.895 -79.252 117.575  1.00 39.79      A
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ATOM   1632  CD2 PHE A 329     240.097 -78.138 115.808  1.00 39.80      A
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ATOM   1633  CE1 PHE A 329     237.824 -79.529 116.665  1.00 42.28      A
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ATOM   1634  CE2 PHE A 329     239.034 -78.408 114.902  1.00 45.87      A
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ATOM   1635  CZ  PHE A 329     237.903 -79.106 115.332  1.00 40.12      A
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ATOM   1636  C   PHE A 329     241.904 -76.978 120.064  1.00 45.73      A
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ATOM   1637  O   PHE A 329     242.769 -77.808 120.277  1.00 40.30      A
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ATOM   1672  CE1 TYR A 334     252.454 -82.152 117.323  1.00 57.12      A
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ATOM   1673  CD2 TYR A 334     251.556 -83.561 119.454  1.00 60.46      A
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C
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ATOM   1695  CB  THR A 337     246.221 -79.805 120.292  1.00 48.60      A
C
ATOM   1696  OG1 THR A 337     246.433 -78.730 121.227  1.00 44.49      A
O
ATOM   1697  CG2 THR A 337     245.691 -79.262 118.948  1.00 33.80      A
C
ATOM   1698  C   THR A 337     245.031 -81.916 119.825  1.00 55.74      A
C
ATOM   1699  O   THR A 337     244.036 -81.911 119.094  1.00 53.43      A
O
ATOM   1700  N   TYR A 338     245.979 -82.848 119.758  1.00 62.69      A
N
ATOM   1701  CA  TYR A 338     245.902 -83.948 118.795  1.00 62.09      A
C
ATOM   1702  CB  TYR A 338     247.056 -84.923 119.028  1.00 70.33      A
C
ATOM   1703  CG  TYR A 338     247.098 -86.080 118.034  1.00 74.69      A
C
ATOM   1704  CD1 TYR A 338     248.041 -86.116 117.016  1.00 72.79      A
C
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ATOM   1705  CE1 TYR A 338     248.050 -87.154 116.101  1.00 75.92      A
C
ATOM   1706  CD2 TYR A 338     246.167 -87.121 118.096  1.00 70.94      A
C
ATOM   1707  CE2 TYR A 338     246.167 -88.153 117.173  1.00 73.14      A
C
ATOM   1708  CZ  TYR A 338     247.102 -88.168 116.186  1.00 73.24      A
C
ATOM   1709  OH  TYR A 338     247.091 -89.196 115.273  1.00 74.46      A
O
ATOM   1710  C   TYR A 338     244.586 -84.698 118.971  1.00 62.03      A
C
ATOM   1711  O   TYR A 338     243.884 -85.017 117.982  1.00 52.46      A
O
ATOM   1712  N   LYS A 339     244.267 -84.991 120.242  1.00 58.53      A
N
ATOM   1713  CA  LYS A 339     243.048 -85.733 120.587  1.00 51.87      A
C
ATOM   1714  CB  LYS A 339     243.020 -86.042 122.063  1.00 52.84      A
C
ATOM   1715  C   LYS A 339     241.791 -84.990 120.165  1.00 50.97      A
C
ATOM   1716  O   LYS A 339     240.975 -85.531 119.412  1.00 50.87      A
O
ATOM   1717  N   ARG A 340     241.675 -83.725 120.575  1.00 44.05      A
N
ATOM   1718  CA  ARG A 340     240.507 -82.938 120.230  1.00 47.22      A
C
ATOM   1719  CB  ARG A 340     240.532 -81.574 120.904  1.00 45.76      A
C
ATOM   1720  CG  ARG A 340     240.286 -81.607 122.398  1.00 52.85      A
C
ATOM   1721  CD  ARG A 340     240.241 -80.202 122.999  1.00 59.79      A
C
ATOM   1722  NE  ARG A 340     239.045 -79.491 122.535  1.00 67.64      A
N
ATOM   1723  CZ  ARG A 340     238.843 -78.186 122.672  1.00 65.86      A
C
ATOM   1724  NH1 ARG A 340     239.763 -77.446 123.254  1.00 67.71      A
N
ATOM   1725  NH2 ARG A 340     237.722 -77.631 122.240  1.00 68.60      A
N
ATOM   1726  C   ARG A 340     240.299 -82.765 118.738  1.00 46.20      A
C
ATOM   1727  O   ARG A 340     239.144 -82.785 118.274  1.00 48.74      A
O
ATOM   1728  N   ILE A 341     241.387 -82.597 117.979  1.00 47.52      A
N
ATOM   1729  CA  ILE A 341     241.253 -82.462 116.511  1.00 49.01      A
C
ATOM   1730  CB  ILE A 341     242.586 -82.067 115.787  1.00 48.35      A
C
ATOM   1731  CG2 ILE A 341     242.367 -82.130 114.290  1.00 34.18      A
C
ATOM   1732  CG1 ILE A 341     243.053 -80.674 116.236  1.00 44.80      A
C
ATOM   1733  CD1 ILE A 341     244.317 -80.259 115.592  1.00 47.34      A
C
ATOM   1734  C   ILE A 341     240.783 -83.752 115.851  1.00 53.55      A
C
ATOM   1735  O   ILE A 341     239.936 -83.734 114.948  1.00 44.79      A
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ATOM	1736	N	SER	A	342	241.369	-84.867	116.286	1.00	59.31	A
N											
ATOM	1737	CA	SER	A	342	241.014	-86.175	115.743	1.00	65.95	A
C											
ATOM	1738	CB	SER	A	342	242.037	-87.227	116.158	1.00	66.33	A
C											
ATOM	1739	OG	SER	A	342	241.613	-88.516	115.745	1.00	63.35	A
O											
ATOM	1740	C	SER	A	342	239.628	-86.604	116.202	1.00	65.99	A
C											
ATOM	1741	O	SER	A	342	238.941	-87.327	115.475	1.00	61.18	A
O											
ATOM	1742	N	ARG	A	343	239.232	-86.162	117.400	1.00	61.34	A
N											
ATOM	1743	CA	ARG	A	343	237.910	-86.478	117.932	1.00	59.46	A
C											
ATOM	1744	CB	ARG	A	343	237.888	-86.410	119.456	1.00	58.77	A
C											
ATOM	1745	CG	ARG	A	343	238.466	-87.604	120.201	1.00	47.50	A
C											
ATOM	1746	CD	ARG	A	343	238.360	-87.314	121.675	1.00	60.64	A
C											
ATOM	1747	NE	ARG	A	343	238.972	-88.327	122.530	1.00	66.55	A
N											
ATOM	1748	CZ	ARG	A	343	238.930	-88.278	123.865	1.00	74.36	A
C											
ATOM	1749	NH1	ARG	A	343	238.309	-87.268	124.510	1.00	73.84	A
N											
ATOM	1750	NH2	ARG	A	343	239.502	-89.248	124.573	1.00	82.35	A
N											
ATOM	1751	C	ARG	A	343	236.902	-85.448	117.406	1.00	62.95	A
C											
ATOM	1752	O	ARG	A	343	235.682	-85.706	117.372	1.00	61.25	A
O											
ATOM	1753	N	VAL	A	344	237.421	-84.275	117.011	1.00	62.37	A
N											
ATOM	1754	CA	VAL	A	344	236.592	-83.163	116.517	1.00	52.53	A
C											
ATOM	1755	CB	VAL	A	344	235.625	-83.614	115.386	1.00	46.83	A
C											
ATOM	1756	CG1	VAL	A	344	235.005	-82.383	114.685	1.00	30.17	A
C											
ATOM	1757	CG2	VAL	A	344	236.378	-84.445	114.375	1.00	41.05	A
C											
ATOM	1758	C	VAL	A	344	235.794	-82.735	117.737	1.00	56.35	A
C											
ATOM	1759	O	VAL	A	344	234.569	-82.790	117.750	1.00	58.20	A
O											
ATOM	1760	N	GLU	A	345	236.521	-82.345	118.775	1.00	52.70	A
N											
ATOM	1761	CA	GLU	A	345	235.945	-81.929	120.037	1.00	55.50	A
C											
ATOM	1762	CB	GLU	A	345	236.726	-82.610	121.170	1.00	59.39	A
C											
ATOM	1763	CG	GLU	A	345	236.049	-82.656	122.512	1.00	70.94	A
C											
ATOM	1764	CD	GLU	A	345	236.741	-83.623	123.456	1.00	80.37	A
C											
ATOM	1765	OE1	GLU	A	345	236.904	-84.815	123.076	1.00	83.68	A
O											
ATOM	1766	OE2	GLU	A	345	237.114	-83.190	124.572	1.00	84.85	A
O											

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ATOM   1767  C   GLU A 345     235.984 -80.414 120.226  1.00 55.94      A
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ATOM   1768  O   GLU A 345     237.012 -79.866 120.647  1.00 52.34      A
O
ATOM   1769  N   PHE A 346     234.868 -79.746 119.941  1.00 55.31      A
N
ATOM   1770  CA  PHE A 346     234.777 -78.298 120.123  1.00 58.97      A
C
ATOM   1771  CB  PHE A 346     235.238 -77.601 118.840  1.00 55.59      A
C
ATOM   1772  CG  PHE A 346     234.247 -77.671 117.721  1.00 51.30      A
C
ATOM   1773  CD1 PHE A 346     233.315 -76.667 117.540  1.00 47.92      A
C
ATOM   1774  CD2 PHE A 346     234.261 -78.734 116.842  1.00 51.74      A
C
ATOM   1775  CE1 PHE A 346     232.396 -76.715 116.483  1.00 54.03      A
C
ATOM   1776  CE2 PHE A 346     233.348 -78.810 115.764  1.00 54.32      A
C
ATOM   1777  CZ  PHE A 346     232.409 -77.803 115.575  1.00 51.48      A
C
ATOM   1778  C   PHE A 346     233.356 -77.832 120.501  1.00 60.04      A
C
ATOM   1779  O   PHE A 346     232.368 -78.494 120.173  1.00 69.92      A
O
ATOM   1780  N   THR A 347     233.261 -76.697 121.184  1.00 56.17      A
N
ATOM   1781  CA  THR A 347     231.979 -76.158 121.555  1.00 54.44      A
C
ATOM   1782  CB  THR A 347     231.732 -76.329 123.013  1.00 47.09      A
C
ATOM   1783  OG1 THR A 347     232.718 -75.600 123.725  1.00 47.43      A
O
ATOM   1784  CG2 THR A 347     231.799 -77.783 123.402  1.00 48.24      A
C
ATOM   1785  C   THR A 347     231.885 -74.683 121.223  1.00 56.33      A
C
ATOM   1786  O   THR A 347     232.902 -73.985 121.113  1.00 62.80      A
O
ATOM   1787  N   PHE A 348     230.646 -74.235 120.999  1.00 63.69      A
N
ATOM   1788  CA  PHE A 348     230.389 -72.815 120.723  1.00 65.89      A
C
ATOM   1789  CB  PHE A 348     229.306 -72.558 119.708  1.00 57.72      A
C
ATOM   1790  CG  PHE A 348     229.584 -73.148 118.381  1.00 55.81      A
C
ATOM   1791  CD1 PHE A 348     229.017 -74.364 118.020  1.00 51.99      A
C
ATOM   1792  CD2 PHE A 348     230.337 -72.462 117.450  1.00 53.67      A
C
ATOM   1793  CE1 PHE A 348     229.171 -74.857 116.780  1.00 46.52      A
C
ATOM   1794  CE2 PHE A 348     230.492 -72.966 116.190  1.00 50.86      A
C
ATOM   1795  CZ  PHE A 348     229.903 -74.166 115.860  1.00 51.38      A
C
ATOM   1796  C   PHE A 348     229.966 -72.048 121.961  1.00 65.81      A
C
ATOM   1797  O   PHE A 348     229.223 -72.532 122.808  1.00 73.51      A
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ATOM 1798 N PRO A 349 230.578 -70.898 122.150 1.00 59.06 A
N
ATOM 1799 CD PRO A 349 232.018 -71.026 121.861 1.00 61.27 A
C
ATOM 1800 CA PRO A 349 230.381 -69.933 123.199 1.00 56.66 A
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ATOM 1801 CB PRO A 349 231.466 -68.944 122.870 1.00 58.77 A
C
ATOM 1802 CG PRO A 349 232.627 -69.875 122.485 1.00 55.14 A
C
ATOM 1803 C PRO A 349 228.929 -69.409 122.948 1.00 57.97 A
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ATOM 1804 O PRO A 349 228.312 -69.642 121.916 1.00 59.47 A
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ATOM 1805 N ASP A 350 228.344 -68.735 123.909 1.00 59.19 A
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ATOM 1806 CA ASP A 350 226.961 -68.282 123.714 1.00 51.98 A
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ATOM 1807 CB ASP A 350 226.338 -67.819 125.044 1.00 65.27 A
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ATOM 1808 CG ASP A 350 226.140 -68.958 126.020 1.00 72.68 A
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ATOM 1809 OD1 ASP A 350 225.764 -68.668 127.188 1.00 77.91 A
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ATOM 1810 OD2 ASP A 350 226.359 -70.131 125.607 1.00 78.14 A
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ATOM 1811 C ASP A 350 226.787 -67.197 122.665 1.00 54.69 A
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ATOM 1812 O ASP A 350 225.753 -67.202 121.947 1.00 40.28 A
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ATOM 1813 N PHE A 351 227.786 -66.308 122.539 1.00 47.45 A
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ATOM 1814 CA PHE A 351 227.682 -65.217 121.584 1.00 51.83 A
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ATOM 1815 CB PHE A 351 228.693 -64.106 121.893 1.00 48.14 A
C
ATOM 1816 CG PHE A 351 230.108 -64.580 122.004 1.00 51.21 A
C
ATOM 1817 CD1 PHE A 351 230.589 -65.111 123.207 1.00 49.73 A
C
ATOM 1818 CD2 PHE A 351 230.979 -64.468 120.915 1.00 46.79 A
C
ATOM 1819 CE1 PHE A 351 231.906 -65.506 123.312 1.00 48.51 A
C
ATOM 1820 CE2 PHE A 351 232.294 -64.864 121.026 1.00 47.18 A
C
ATOM 1821 CZ PHE A 351 232.758 -65.379 122.215 1.00 45.61 A
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ATOM 1822 C PHE A 351 227.797 -65.610 120.125 1.00 52.56 A
C
ATOM 1823 O PHE A 351 227.604 -64.771 119.250 1.00 57.29 A
O
ATOM 1824 N VAL A 352 228.115 -66.874 119.863 1.00 54.95 A
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ATOM 1825 CA VAL A 352 228.263 -67.341 118.495 1.00 48.00 A
C
ATOM 1826 CB VAL A 352 229.145 -68.621 118.432 1.00 43.19 A
C
ATOM 1827 CG1 VAL A 352 229.300 -69.094 117.035 1.00 33.61 A
C
ATOM 1828 CG2 VAL A 352 230.509 -68.325 118.972 1.00 39.08 A
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ATOM   1829  C   VAL A 352     226.875 -67.603 117.916  1.00 48.25      A
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ATOM   1830  O   VAL A 352     226.211 -68.567 118.255  1.00 51.46      A
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N
ATOM   1832  CA  THR A 353     225.122 -66.886 116.413  1.00 53.02      A
C
ATOM   1833  CB  THR A 353     224.844 -65.817 115.383  1.00 47.94      A
C
ATOM   1834  OG1 THR A 353     225.671 -66.052 114.246  1.00 54.22      A
O
ATOM   1835  CG2 THR A 353     225.130 -64.437 115.950  1.00 47.89      A
C
ATOM   1836  C   THR A 353     224.908 -68.227 115.753  1.00 52.60      A
C
ATOM   1837  O   THR A 353     225.851 -68.974 115.552  1.00 52.94      A
O
ATOM   1838  N   GLU A 354     223.654 -68.513 115.404  1.00 55.25      A
N
ATOM   1839  CA  GLU A 354     223.259 -69.786 114.819  1.00 56.40      A
C
ATOM   1840  CB  GLU A 354     221.736 -69.929 114.829  1.00 53.45      A
C
ATOM   1841  C   GLU A 354     223.762 -69.866 113.416  1.00 56.12      A
C
ATOM   1842  O   GLU A 354     224.078 -70.954 112.927  1.00 62.85      A
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ATOM   1843  N   GLY A 355     223.831 -68.718 112.749  1.00 61.99      A
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ATOM   1844  CA  GLY A 355     224.317 -68.699 111.373  1.00 52.27      A
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ATOM   1845  C   GLY A 355     225.787 -69.093 111.250  1.00 52.90      A
C
ATOM   1846  O   GLY A 355     226.166 -69.822 110.327  1.00 47.53      A
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ATOM   1847  N   ALA A 356     226.611 -68.602 112.182  1.00 47.86      A
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ATOM   1848  CA  ALA A 356     228.022 -68.912 112.199  1.00 45.96      A
C
ATOM   1849  CB  ALA A 356     228.721 -67.995 113.123  1.00 42.05      A
C
ATOM   1850  C   ALA A 356     228.221 -70.359 112.627  1.00 47.72      A
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ATOM   1854  CB  ARG A 357     226.549 -72.374 115.280  1.00 55.71      A
C
ATOM   1855  CG  ARG A 357     226.876 -71.606 116.583  1.00 57.21      A
C
ATOM   1856  CD  ARG A 357     226.018 -72.108 117.752  1.00 41.40      A
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ATOM   1857  NE  ARG A 357     226.260 -71.310 118.928  1.00 43.14      A
N
ATOM   1858  CZ  ARG A 357     225.979 -71.698 120.148  1.00 39.58      A
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ATOM   1859  NH1 ARG A 357     225.456 -72.893 120.340  1.00 42.66      A
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ATOM   1860  NH2 ARG A 357     226.191 -70.869 121.163  1.00 51.41      A
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ATOM   1861  C   ARG A 357     227.299 -73.181 113.043  1.00 58.61      A
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ATOM   1862  O   ARG A 357     227.922 -74.260 112.996  1.00 62.70      A
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ATOM   1863  N   ASP A 358     226.383 -72.845 112.150  1.00 56.80      A
N
ATOM   1864  CA  ASP A 358     226.053 -73.738 111.055  1.00 56.49      A
C
ATOM   1865  CB  ASP A 358     224.792 -73.245 110.363  1.00 59.12      A
C
ATOM   1866  CG  ASP A 358     224.380 -74.141 109.209  1.00 65.41      A
C
ATOM   1867  OD1 ASP A 358     224.036 -75.319 109.461  1.00 60.89      A
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ATOM   1868  OD2 ASP A 358     224.403 -73.669 108.049  1.00 68.71      A
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ATOM   1869  C   ASP A 358     227.178 -73.837 110.017  1.00 56.31      A
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C
ATOM   1874  CG  LEU A 359     230.326 -71.029 107.344  1.00 49.10      A
C
ATOM   1875  CD1 LEU A 359     230.077 -71.756 106.082  1.00 42.56      A
C
ATOM   1876  CD2 LEU A 359     230.525 -69.538 107.083  1.00 51.15      A
C
ATOM   1877  C   LEU A 359     230.048 -73.366 109.200  1.00 57.66      A
C
ATOM   1878  O   LEU A 359     230.680 -74.142 108.481  1.00 65.55      A
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C
ATOM   1881  CB  ILE A 360     231.819 -73.111 112.485  1.00 35.85      A
C
ATOM   1882  CG2 ILE A 360     232.892 -73.858 113.220  1.00 37.90      A
C
ATOM   1883  CG1 ILE A 360     232.254 -71.652 112.301  1.00 32.36      A
C
ATOM   1884  CD1 ILE A 360     232.250 -70.839 113.653  1.00 27.28      A
C
ATOM   1885  C   ILE A 360     231.368 -75.240 111.229  1.00 40.84      A
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ATOM   1887  N   SER A 361     230.158 -75.670 111.591  1.00 46.60      A
N
ATOM   1888  CA  SER A 361     229.855 -77.089 111.780  1.00 52.65      A
C
ATOM   1889  CB  SER A 361     228.546 -77.265 112.526  1.00 49.78      A
C
ATOM   1890  OG  SER A 361     228.742 -77.062 113.925  1.00 60.97      A
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ATOM   1891  C   SER A 361     229.827 -77.906 110.497  1.00 53.49      A
C
ATOM   1892  O   SER A 361     229.885 -79.159 110.538  1.00 53.09      A
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ATOM   1893  N   ARG A 362     229.799 -77.198 109.368  1.00 54.39      A
N
ATOM   1894  CA  ARG A 362     229.796 -77.841 108.066  1.00 52.12      A
C
ATOM   1895  CB  ARG A 362     229.033 -76.978 107.065  1.00 59.93      A
C
ATOM   1896  CG  ARG A 362     227.535 -76.862 107.327  1.00 61.75      A
C
ATOM   1897  CD  ARG A 362     226.887 -75.820 106.401  1.00 69.51      A
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ATOM   1898  NE  ARG A 362     225.432 -75.784 106.547  1.00 76.19      A
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ATOM   1899  CZ  ARG A 362     224.625 -76.795 106.216  1.00 80.23      A
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ATOM   1902  C   ARG A 362     231.211 -78.066 107.537  1.00 49.26      A
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ATOM   1903  O   ARG A 362     231.460 -79.036 106.822  1.00 49.03      A
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ATOM   1904  N   LEU A 363     232.120 -77.162 107.891  1.00 49.05      A
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ATOM   1905  CA  LEU A 363     233.493 -77.234 107.438  1.00 46.81      A
C
ATOM   1906  CB  LEU A 363     234.134 -75.850 107.508  1.00 42.60      A
C
ATOM   1907  CG  LEU A 363     233.457 -74.729 106.714  1.00 44.53      A
C
ATOM   1908  CD1 LEU A 363     234.050 -73.356 107.133  1.00 43.18      A
C
ATOM   1909  CD2 LEU A 363     233.602 -74.961 105.258  1.00 42.47      A
C
ATOM   1910  C   LEU A 363     234.270 -78.228 108.280  1.00 49.03      A
C
ATOM   1911  O   LEU A 363     235.049 -79.020 107.751  1.00 57.90      A
O
ATOM   1912  N   LEU A 364     234.062 -78.186 109.589  1.00 47.92      A
N
ATOM   1913  CA  LEU A 364     234.774 -79.071 110.488  1.00 49.66      A
C
ATOM   1914  CB  LEU A 364     234.792 -78.462 111.909  1.00 46.24      A
C
ATOM   1915  CG  LEU A 364     235.511 -77.115 112.043  1.00 47.59      A
C
ATOM   1916  CD1 LEU A 364     235.230 -76.547 113.413  1.00 44.59      A
C
ATOM   1917  CD2 LEU A 364     237.029 -77.318 111.836  1.00 45.40      A
C
ATOM   1918  C   LEU A 364     234.233 -80.493 110.526  1.00 50.53      A
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ATOM   1919  O   LEU A 364     233.804 -80.963 111.575  1.00 56.94      A
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ATOM   1920  N   LYS A 365     234.267 -81.178 109.385  1.00 61.00      A
N
ATOM   1921  CA  LYS A 365     233.796 -82.564 109.263  1.00 64.52      A
C
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ATOM   1922  CB  LYS A 365     233.059 -82.728 107.925  1.00 60.48      A
C
ATOM   1923  CG  LYS A 365     231.753 -81.921 107.829  1.00 53.27      A
C
ATOM   1924  CD  LYS A 365     230.702 -82.412 108.828  1.00 61.58      A
C
ATOM   1925  CE  LYS A 365     229.295 -81.895 108.447  1.00 59.92      A
C
ATOM   1926  NZ  LYS A 365     228.297 -82.223 109.508  1.00 75.42      A
N
ATOM   1927  C   LYS A 365     235.026 -83.500 109.392  1.00 66.56      A
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ATOM   1929  N   HIS A 366     234.844 -84.748 109.813  1.00 68.20      A
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ATOM   1931  CB  HIS A 366     235.781 -86.664 111.109  1.00 66.12      A
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ATOM   1932  CG  HIS A 366     236.913 -87.628 111.242  1.00 68.47      A
C
ATOM   1933  CD2 HIS A 366     237.810 -87.749 112.245  1.00 66.88      A
C
ATOM   1934  ND1 HIS A 366     237.332 -88.487 110.238  1.00 66.01      A
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ATOM   1935  CE1 HIS A 366     238.454 -89.075 110.623  1.00 70.20      A
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ATOM   1936  NE2 HIS A 366     238.761 -88.643 111.832  1.00 64.97      A
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ATOM   1937  C   HIS A 366     236.184 -86.385 108.739  1.00 68.25      A
C
ATOM   1938  O   HIS A 366     237.098 -87.249 108.572  1.00 74.87      A
O
ATOM   1939  N   ASN A 367     235.262 -86.111 107.848  1.00 65.45      A
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ATOM   1940  CA  ASN A 367     235.379 -86.795 106.656  1.00 62.81      A
C
ATOM   1941  CB  ASN A 367     234.189 -87.664 106.498  1.00 64.61      A
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ATOM   1942  CG  ASN A 367     234.335 -88.548 105.333  1.00 69.77      A
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ATOM   1943  OD1 ASN A 367     234.339 -88.071 104.175  1.00 65.35      A
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ATOM   1944  ND2 ASN A 367     234.518 -89.855 105.596  1.00 69.27      A
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ATOM   1945  C   ASN A 367     235.504 -85.791 105.596  1.00 60.17      A
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ATOM   1946  O   ASN A 367     234.685 -84.923 105.475  1.00 67.65      A
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ATOM   1948  CD  PRO A 368     237.882 -86.364 105.504  1.00 55.35      A
C
ATOM   1949  CA  PRO A 368     236.981 -84.895 103.820  1.00 55.82      A
C
ATOM   1950  CB  PRO A 368     238.199 -85.537 103.245  1.00 50.93      A
C
ATOM   1951  CG  PRO A 368     238.938 -85.936 104.468  1.00 54.85      A
C
ATOM   1952  C   PRO A 368     235.870 -84.741 102.783  1.00 59.90      A
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ATOM 1953 O PRO A 368 235.706 -83.658 102.240 1.00 61.00 A
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ATOM 1954 N SER A 369 235.093 -85.805 102.557 1.00 69.67 A
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ATOM 1955 CA SER A 369 234.000 -85.800 101.588 1.00 72.88 A
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ATOM 1956 CB SER A 369 233.537 -87.237 101.347 1.00 75.22 A
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ATOM 1957 OG SER A 369 234.654 -88.115 101.256 1.00 85.92 A
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ATOM 1958 C SER A 369 232.810 -84.951 102.046 1.00 71.84 A
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ATOM 1959 O SER A 369 232.217 -84.231 101.229 1.00 75.53 A
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ATOM 1960 N GLN A 370 232.465 -85.039 103.333 1.00 67.85 A
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ATOM 1961 CA GLN A 370 231.339 -84.296 103.865 1.00 62.69 A
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ATOM 1962 CB GLN A 370 231.067 -84.743 105.296 1.00 64.15 A
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ATOM 1963 CG GLN A 370 230.629 -86.190 105.390 1.00 65.40 A
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ATOM 1964 CD GLN A 370 230.923 -86.768 106.745 1.00 69.41 A
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ATOM 1965 OE1 GLN A 370 230.904 -86.051 107.752 1.00 75.34 A
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ATOM 1968 O GLN A 370 230.582 -82.028 103.608 1.00 65.90 A
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ATOM 1971 CB ARG A 371 234.581 -80.691 103.961 1.00 48.64 A
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ATOM 1972 CG ARG A 371 235.109 -80.785 105.354 1.00 46.61 A
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ATOM 1973 CD ARG A 371 236.618 -80.922 105.403 1.00 43.30 A
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ATOM 1974 NE ARG A 371 236.988 -81.971 106.350 1.00 42.51 A
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ATOM 1975 CZ ARG A 371 238.208 -82.476 106.436 1.00 42.45 A
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ATOM 1976 NH1 ARG A 371 239.165 -81.997 105.635 1.00 36.24 A
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ATOM 1977 NH2 ARG A 371 238.449 -83.494 107.266 1.00 33.74 A
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ATOM 1978 C ARG A 371 232.496 -80.275 102.651 1.00 56.25 A
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ATOM 1979 O ARG A 371 232.578 -80.836 101.587 1.00 64.77 A
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ATOM 1982 CA PRO A 372 231.260 -78.365 101.659 1.00 57.19 A
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ATOM 1983 CB PRO A 372 230.522 -77.231 102.348 1.00 55.89 A
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ATOM   1987  N   MET A 373     231.685 -77.356  99.497  1.00 66.48      A
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ATOM   1988  CA  MET A 373     232.482 -76.838  98.412  1.00 72.53      A
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ATOM   1989  CB  MET A 373     231.763 -77.051  97.082  1.00 78.23      A
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ATOM   1990  CG  MET A 373     232.541 -77.969  96.165  1.00 91.60      A
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ATOM   1991  SD  MET A 373     231.857 -78.033  94.463  1.00 92.28      A
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ATOM   1992  CE  MET A 373     230.337 -78.924  94.769  1.00 97.23      A
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ATOM   1993  C   MET A 373     232.631 -75.339  98.682  1.00 69.48      A
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ATOM   1994  O   MET A 373     231.861 -74.740  99.424  1.00 71.05      A
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ATOM   1995  N   LEU A 374     233.618 -74.722  98.060  1.00 66.97      A
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ATOM   1996  CA  LEU A 374     233.847 -73.303  98.261  1.00 65.90      A
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ATOM   1997  CB  LEU A 374     235.155 -72.857  97.562  1.00 58.73      A
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ATOM   1998  CG  LEU A 374     236.446 -73.311  98.258  1.00 51.64      A
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ATOM   1999  CD1 LEU A 374     237.625 -73.104  97.321  1.00 47.33      A
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ATOM   2000  CD2 LEU A 374     236.629 -72.531  99.548  1.00 52.27      A
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ATOM   2001  C   LEU A 374     232.660 -72.469  97.798  1.00 67.13      A
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ATOM   2002  O   LEU A 374     232.500 -71.320  98.219  1.00 75.20      A
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C
ATOM   2005  CB  ARG A 375     230.122 -72.780  95.162  1.00 60.43      A
C
ATOM   2006  C   ARG A 375     229.561 -72.275  97.541  1.00 63.36      A
C
ATOM   2007  O   ARG A 375     228.882 -71.261  97.734  1.00 64.17      A
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ATOM   2008  N   GLU A 376     229.413 -73.397  98.245  1.00 56.91      A
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ATOM   2009  CA  GLU A 376     228.404 -73.501  99.306  1.00 64.22      A
C
ATOM   2010  CB  GLU A 376     228.314 -74.947  99.815  1.00 67.11      A
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ATOM   2011  CG  GLU A 376     227.797 -75.921  98.783  1.00 81.78      A
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ATOM   2012  CD  GLU A 376     228.016 -77.372  99.187  1.00 87.25      A
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ATOM   2013  OE1 GLU A 376     229.137 -77.887  98.974  1.00 95.99      A
O
ATOM   2014  OE2 GLU A 376     227.073 -78.001  99.732  1.00 98.67      A
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ATOM 2015 C GLU A 376 228.791 -72.562 100.461 1.00 61.59 A
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ATOM 2016 O GLU A 376 227.950 -72.145 101.275 1.00 63.73 A
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ATOM 2017 N VAL A 377 230.078 -72.229 100.505 1.00 60.90 A
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ATOM 2018 CA VAL A 377 230.605 -71.361 101.539 1.00 60.11 A
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ATOM 2019 CB VAL A 377 232.149 -71.606 101.780 1.00 57.13 A
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ATOM 2020 CG1 VAL A 377 232.701 -70.591 102.788 1.00 52.18 A
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ATOM 2021 CG2 VAL A 377 232.364 -72.987 102.341 1.00 51.22 A
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ATOM 2022 C VAL A 377 230.354 -69.928 101.140 1.00 59.92 A
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ATOM 2023 O VAL A 377 229.915 -69.114 101.952 1.00 69.33 A
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ATOM 2026 CB LEU A 378 231.178 -68.090 98.026 1.00 55.37 A
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ATOM 2027 CG LEU A 378 232.564 -67.442 97.937 1.00 56.77 A
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ATOM 2028 CD1 LEU A 378 232.986 -66.902 99.309 1.00 59.47 A
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ATOM 2029 CD2 LEU A 378 233.517 -68.445 97.421 1.00 52.34 A
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ATOM 2030 C LEU A 378 228.995 -67.925 99.248 1.00 53.77 A
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ATOM 2031 O LEU A 378 228.626 -66.775 99.062 1.00 56.35 A
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ATOM 2032 N GLU A 379 228.144 -68.930 99.367 1.00 58.84 A
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ATOM 2034 CB GLU A 379 226.101 -69.720 98.274 1.00 65.30 A
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ATOM 2035 CG GLU A 379 226.567 -69.569 96.831 1.00 70.53 A
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ATOM 2036 CD GLU A 379 225.831 -70.533 95.895 1.00 76.21 A
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ATOM 2037 OE1 GLU A 379 225.546 -71.692 96.329 1.00 70.09 A
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ATOM 2038 OE2 GLU A 379 225.547 -70.124 94.737 1.00 76.09 A
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ATOM 2039 C GLU A 379 225.991 -68.820 100.555 1.00 60.26 A
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ATOM 2040 O GLU A 379 224.963 -68.191 100.746 1.00 70.86 A
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ATOM 2041 N HIS A 380 226.535 -69.606 101.468 1.00 54.34 A
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ATOM 2042 CA HIS A 380 225.921 -69.775 102.771 1.00 54.61 A
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ATOM 2043 CB HIS A 380 226.975 -70.234 103.793 1.00 48.39 A
C
ATOM 2044 CG HIS A 380 226.402 -70.617 105.121 1.00 45.24 A
C
ATOM 2045 CD2 HIS A 380 226.402 -71.793 105.781 1.00 42.14 A
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ATOM   2046  ND1 HIS A 380     225.711 -69.731 105.921  1.00 51.46      A
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ATOM   2047  CE1 HIS A 380     225.309 -70.349 107.018  1.00 50.88      A
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ATOM   2048  NE2 HIS A 380     225.715 -71.604 106.957  1.00 47.24      A
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ATOM   2049  C   HIS A 380     225.231 -68.502 103.261  1.00 55.95      A
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ATOM   2050  O   HIS A 380     225.807 -67.409 103.206  1.00 60.83      A
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C
ATOM   2053  CA  PRO A 381     223.147 -67.522 104.248  1.00 53.48      A
C
ATOM   2054  CB  PRO A 381     221.997 -68.257 104.936  1.00 49.53      A
C
ATOM   2055  CG  PRO A 381     221.820 -69.442 104.035  1.00 49.24      A
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ATOM   2056  C   PRO A 381     223.875 -66.545 105.212  1.00 56.98      A
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ATOM   2057  O   PRO A 381     223.758 -65.320 105.074  1.00 59.03      A
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ATOM   2058  N   TRP A 382     224.635 -67.091 106.164  1.00 54.77      A
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ATOM   2061  CG  TRP A 382     226.691 -66.368 109.261  1.00 55.47      A
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ATOM   2062  CD2 TRP A 382     228.111 -66.195 109.372  1.00 58.05      A
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ATOM   2063  CE2 TRP A 382     228.344 -65.342 110.476  1.00 60.80      A
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ATOM   2064  CE3 TRP A 382     229.210 -66.680 108.649  1.00 60.95      A
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ATOM   2065  CD1 TRP A 382     226.137 -65.634 110.266  1.00 58.89      A
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ATOM   2066  NE1 TRP A 382     227.123 -65.011 111.004  1.00 59.37      A
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ATOM   2067  CZ2 TRP A 382     229.632 -64.965 110.871  1.00 64.01      A
C
ATOM   2068  CZ3 TRP A 382     230.491 -66.302 109.042  1.00 60.80      A
C
ATOM   2069  CH2 TRP A 382     230.688 -65.458 110.140  1.00 65.05      A
C
ATOM   2070  C   TRP A 382     226.397 -65.476 106.455  1.00 50.36      A
C
ATOM   2071  O   TRP A 382     226.579 -64.300 106.749  1.00 56.46      A
O
ATOM   2072  N   ILE A 383     227.094 -66.115 105.527  1.00 50.17      A
N
ATOM   2073  CA  ILE A 383     228.163 -65.454 104.757  1.00 51.21      A
C
ATOM   2074  CB  ILE A 383     228.914 -66.460 103.856  1.00 42.86      A
C
ATOM   2075  CG2 ILE A 383     229.642 -65.709 102.766  1.00 42.15      A
C
ATOM   2076  CG1 ILE A 383     229.846 -67.329 104.708  1.00 40.04      A
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ATOM   2077  CD1 ILE A 383     230.943 -66.520 105.429  1.00 40.46      A
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ATOM   2078  C   ILE A 383     227.659 -64.305 103.873  1.00 52.36      A
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N
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C
ATOM   2082  CB  THR A 384     225.046 -64.197 101.265  1.00 57.25      A
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ATOM   2084  CG2 THR A 384     225.809 -64.804 100.133  1.00 59.94      A
C
ATOM   2085  C   THR A 384     225.221 -62.436 102.988  1.00 57.62      A
C
ATOM   2086  O   THR A 384     224.929 -61.395 102.420  1.00 61.64      A
O
ATOM   2087  N   ALA A 385     224.911 -62.655 104.249  1.00 60.34      A
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ATOM   2088  CA  ALA A 385     224.195 -61.658 105.030  1.00 57.14      A
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ATOM   2089  CB  ALA A 385     223.197 -62.376 105.944  1.00 61.04      A
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ATOM   2090  C   ALA A 385     225.112 -60.735 105.867  1.00 57.68      A
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ATOM   2091  O   ALA A 385     224.644 -59.765 106.467  1.00 56.76      A
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ATOM   2093  CA  ASN A 386     227.312 -60.217 106.705  1.00 59.50      A
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ATOM   2094  CB  ASN A 386     227.751 -60.993 107.939  1.00 58.18      A
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ATOM   2095  CG  ASN A 386     226.583 -61.313 108.874  1.00 60.78      A
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ATOM   2096  OD1 ASN A 386     226.026 -60.419 109.536  1.00 55.54      A
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ATOM   2097  ND2 ASN A 386     226.201 -62.591 108.923  1.00 55.70      A
N
ATOM   2098  C   ASN A 386     228.540 -59.733 105.965  1.00 55.04      A
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ATOM   2099  O   ASN A 386     229.128 -58.723 106.336  1.00 58.67      A
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ATOM   2100  N   SER A 387     228.903 -60.444 104.906  1.00 58.95      A
N
ATOM   2101  CA  SER A 387     230.095 -60.110 104.132  1.00 63.83      A
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ATOM   2102  CB  SER A 387     230.472 -61.278 103.220  1.00 55.03      A
C
ATOM   2103  OG  SER A 387     231.719 -61.061 102.599  1.00 57.80      A
O
ATOM   2104  C   SER A 387     229.865 -58.867 103.278  1.00 64.86      A
C
ATOM   2105  O   SER A 387     228.745 -58.607 102.826  1.00 68.20      A
O
ATOM   2106  N   SER A 388     230.916 -58.091 103.063  1.00 67.77      A
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ATOM   2107  CA  SER A 388     230.786 -56.912 102.251  1.00 71.39      A
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ATOM	2108	CB	SER	A	388	231.430	-55.722	102.969	1.00	71.24	A
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ATOM	2109	OG	SER	A	388	232.815	-55.916	103.141	1.00	79.50	A
O											
ATOM	2110	C	SER	A	388	231.403	-57.150	100.872	1.00	71.24	A
C											
ATOM	2111	O	SER	A	388	231.024	-56.501	99.909	1.00	76.22	A
O											
ATOM	2112	N	LYS	A	389	232.336	-58.091	100.767	1.00	70.18	A
N											
ATOM	2113	CA	LYS	A	389	232.951	-58.347	99.475	1.00	67.46	A
C											
ATOM	2114	CB	LYS	A	389	234.459	-58.686	99.667	1.00	49.89	A
C											
ATOM	2115	C	LYS	A	389	232.216	-59.459	98.688	1.00	68.81	A
C											
ATOM	2116	O	LYS	A	389	231.441	-60.236	99.337	1.00	76.61	A
O											
ATOM	2117	OXT	LYS	A	389	232.453	-59.564	97.435	1.00	76.72	A
O											
ATOM	2118	PB	ADP	S	531	257.416	-68.553	107.649	1.00	34.84	S
P											
ATOM	2119	O1B	ADP	S	531	258.545	-67.776	107.191	1.00	50.81	S
O											
ATOM	2120	O2B	ADP	S	531	257.209	-69.880	106.879	1.00	48.35	S
O											
ATOM	2121	O3B	ADP	S	531	257.422	-68.756	109.226	1.00	53.79	S
O											
ATOM	2122	PA	ADP	S	531	256.077	-66.204	106.616	1.00	35.25	S
P											
ATOM	2123	O1A	ADP	S	531	256.842	-66.123	105.373	1.00	33.66	S
O											
ATOM	2124	O2A	ADP	S	531	254.551	-65.860	106.461	1.00	54.13	S
O											
ATOM	2125	O3A	ADP	S	531	256.162	-67.643	107.261	1.00	62.78	S
O											
ATOM	2126	O5*	ADP	S	531	256.892	-65.243	107.657	1.00	48.32	S
O											
ATOM	2127	C5*	ADP	S	531	256.442	-65.218	109.085	1.00	61.70	S
C											
ATOM	2128	C4*	ADP	S	531	255.856	-63.898	109.556	1.00	46.54	S
C											
ATOM	2129	O4*	ADP	S	531	256.542	-62.868	108.818	1.00	44.98	S
O											
ATOM	2130	C3*	ADP	S	531	254.372	-63.620	109.292	1.00	37.55	S
C											
ATOM	2131	O3*	ADP	S	531	253.658	-64.161	110.347	1.00	46.23	S
O											
ATOM	2132	C2*	ADP	S	531	254.337	-62.080	109.181	1.00	46.36	S
C											
ATOM	2133	O2*	ADP	S	531	254.148	-61.399	110.423	1.00	42.59	S
O											
ATOM	2134	C1*	ADP	S	531	255.710	-61.716	108.597	1.00	43.16	S
C											
ATOM	2135	N9	ADP	S	531	255.666	-61.436	107.162	1.00	48.23	S
N											
ATOM	2136	C8	ADP	S	531	255.946	-62.302	106.136	1.00	47.43	S
C											
ATOM	2137	N7	ADP	S	531	255.811	-61.734	104.897	1.00	42.83	S
N											
ATOM	2138	C5	ADP	S	531	255.418	-60.464	105.177	1.00	40.36	S
C											

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ATOM   2139  C6  ADP S 531     255.122 -59.337 104.279  1.00 44.75      S
C
ATOM   2140  N6  ADP S 531     255.151 -59.400 102.949  1.00 22.67      S
N
ATOM   2141  N1  ADP S 531     254.762 -58.153 104.964  1.00 40.38      S
N
ATOM   2142  C2  ADP S 531     254.725 -58.057 106.364  1.00 50.55      S
C
ATOM   2143  N3  ADP S 531     254.992 -59.070 107.188  1.00 51.07      S
N
ATOM   2144  C4  ADP S 531     255.351 -60.245 106.574  1.00 46.49      S
C
ATOM   2145  MG  MG2 X   1     254.502 -68.175 108.413  1.00 47.20      X
MG
ATOM   2146  MG  MG2 X   2     255.864 -71.389 106.282  1.00 52.14      X
MG
ATOM   2147  OH2 WAT W   1     264.531 -71.881  94.078  1.00 38.88      W
O
ATOM   2148  OH2 WAT W   2     242.403 -78.272 113.237  1.00 54.89      W
O
ATOM   2149  OH2 WAT W   3     232.705 -62.634 117.460  1.00 37.08      W
O
ATOM   2150  OH2 WAT W   4     251.977 -73.020 102.685  1.00 62.00      W
O
ATOM   2151  OH2 WAT W   5     275.163 -72.604  97.774  1.00 53.95      W
O
ATOM   2152  OH2 WAT W   6     232.526 -85.909 111.573  1.00 35.05      W
O
ATOM   2153  OH2 WAT W   7     259.170 -71.102 103.608  1.00 40.42      W
O
ATOM   2154  OH2 WAT W   8     249.904 -55.205  99.315  1.00 26.87      W
O
ATOM   2155  OH2 WAT W   9     229.701 -63.236 117.265  1.00 25.50      W
O
```

Table B

ATOM	1	CB	SER	A	123	174.078	193.853	20.627	1.00	33.78	A
C											
ATOM	2	OG	SER	A	123	173.358	193.080	21.584	1.00	34.86	A
O											
ATOM	3	C	SER	A	123	173.331	195.751	21.954	1.00	32.28	A
C											
ATOM	4	O	SER	A	123	174.318	196.187	22.580	1.00	32.38	A
O											
ATOM	5	N	SER	A	123	174.192	196.109	19.556	1.00	32.09	A
N											
ATOM	6	CA	SER	A	123	173.449	195.246	20.532	1.00	33.80	A
C											
ATOM	7	N	LYS	A	124	172.107	195.682	22.463	1.00	30.56	A
N											
ATOM	8	CA	LYS	A	124	171.860	196.059	23.849	1.00	31.07	A
C											
ATOM	9	CB	LYS	A	124	170.483	196.727	24.005	1.00	31.64	A
C											
ATOM	10	CG	LYS	A	124	170.231	197.847	23.021	1.00	33.77	A
C											
ATOM	11	CD	LYS	A	124	168.734	198.157	22.847	1.00	35.14	A
C											
ATOM	12	CE	LYS	A	124	168.571	198.989	21.582	1.00	38.52	A
C											
ATOM	13	NZ	LYS	A	124	167.170	199.182	21.123	1.00	40.74	A
N											
ATOM	14	C	LYS	A	124	171.929	194.785	24.714	1.00	30.29	A
C											
ATOM	15	O	LYS	A	124	171.724	194.845	25.913	1.00	30.99	A
O											
ATOM	16	N	LYS	A	125	172.256	193.646	24.102	1.00	30.71	A
N											
ATOM	17	CA	LYS	A	125	172.352	192.375	24.835	1.00	29.50	A
C											
ATOM	18	CB	LYS	A	125	171.942	191.210	23.951	1.00	32.42	A
C											
ATOM	19	CG	LYS	A	125	170.496	191.147	23.609	1.00	35.74	A
C											
ATOM	20	CD	LYS	A	125	170.221	189.915	22.777	1.00	38.96	A
C											
ATOM	21	CE	LYS	A	125	168.757	189.905	22.351	1.00	44.54	A
C											
ATOM	22	NZ	LYS	A	125	168.305	188.576	21.807	1.00	44.21	A
N											
ATOM	23	C	LYS	A	125	173.728	192.027	25.381	1.00	26.48	A
C											
ATOM	24	O	LYS	A	125	174.769	192.438	24.859	1.00	24.13	A
O											
ATOM	25	N	ARG	A	126	173.713	191.215	26.421	1.00	24.15	A
N											
ATOM	26	CA	ARG	A	126	174.952	190.756	27.020	1.00	22.33	A
C											
ATOM	27	CB	ARG	A	126	174.636	189.835	28.191	1.00	21.13	A
C											
ATOM	28	CG	ARG	A	126	175.841	189.331	28.897	1.00	18.73	A
C											
ATOM	29	CD	ARG	A	126	175.395	188.263	29.847	1.00	19.74	A
C											
ATOM	30	NE	ARG	A	126	176.552	187.628	30.420	1.00	16.73	A
N											

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ATOM     31  CZ  ARG A 126     176.503 186.741  31.394  1.00 17.59      A
C
ATOM     32  NH1 ARG A 126     175.331 186.391  31.902  1.00 16.71      A
N
ATOM     33  NH2 ARG A 126     177.633 186.214  31.854  1.00 18.45      A
N
ATOM     34  C   ARG A 126     175.752 189.995  25.943  1.00 22.44      A
C
ATOM     35  O   ARG A 126     175.252 189.077  25.296  1.00 20.29      A
O
ATOM     36  N   GLN A 127     176.997 190.406  25.763  1.00 21.10      A
N
ATOM     37  CA  GLN A 127     177.904 189.815  24.787  1.00 19.12      A
C
ATOM     38  CB  GLN A 127     178.707 190.934  24.102  1.00 18.99      A
C
ATOM     39  CG  GLN A 127     177.842 191.925  23.355  1.00 15.64      A
C
ATOM     40  CD  GLN A 127     177.154 191.297  22.162  1.00 17.04      A
C
ATOM     41  OE1 GLN A 127     177.748 191.151  21.093  1.00 21.45      A
O
ATOM     42  NE2 GLN A 127     175.902 190.912  22.339  1.00 20.66      A
N
ATOM     43  C   GLN A 127     178.861 188.861  25.496  1.00 17.70      A
C
ATOM     44  O   GLN A 127     179.049 188.941  26.715  1.00 13.46      A
O
ATOM     45  N   TRP A 128     179.460 187.956  24.735  1.00 16.62      A
N
ATOM     46  CA  TRP A 128     180.411 187.014  25.303  1.00 14.25      A
C
ATOM     47  CB  TRP A 128     180.890 186.029  24.237  1.00 13.22      A
C
ATOM     48  CG  TRP A 128     179.858 185.060  23.779  1.00  9.34      A
C
ATOM     49  CD2 TRP A 128     179.264 184.022  24.557  1.00 13.44      A
C
ATOM     50  CE2 TRP A 128     178.396 183.304  23.704  1.00 11.84      A
C
ATOM     51  CE3 TRP A 128     179.389 183.618  25.899  1.00 15.05      A
C
ATOM     52  CD1 TRP A 128     179.338 184.945  22.529  1.00 11.79      A
C
ATOM     53  NE1 TRP A 128     178.460 183.893  22.469  1.00 12.24      A
N
ATOM     54  CZ2 TRP A 128     177.648 182.204  24.146  1.00 10.99      A
C
ATOM     55  CZ3 TRP A 128     178.646 182.523  26.336  1.00 15.81      A
C
ATOM     56  CH2 TRP A 128     177.789 181.828  25.457  1.00 13.35      A
C
ATOM     57  C   TRP A 128     181.611 187.777  25.855  1.00 16.17      A
C
ATOM     58  O   TRP A 128     181.885 188.903  25.457  1.00 17.48      A
O
ATOM     59  N   ALA A 129     182.306 187.146  26.790  1.00 17.52      A
N
ATOM     60  CA  ALA A 129     183.501 187.695  27.415  1.00 17.26      A
C
ATOM     61  CB  ALA A 129     183.129 188.595  28.576  1.00  8.15      A
C
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ATOM     62  C   ALA A 129     184.303 186.478  27.906  1.00 17.06      A
C
ATOM     63  O   ALA A 129     183.733 185.426  28.198  1.00 17.77      A
O
ATOM     64  N   LEU A 130     185.618 186.620  27.979  1.00 16.79      A
N
ATOM     65  CA  LEU A 130     186.479 185.540  28.425  1.00 19.53      A
C
ATOM     66  CB  LEU A 130     187.943 186.006  28.392  1.00 19.86      A
C
ATOM     67  CG  LEU A 130     189.050 184.967  28.619  1.00 22.85      A
C
ATOM     68  CD1 LEU A 130     188.897 183.839  27.604  1.00 17.77      A
C
ATOM     69  CD2 LEU A 130     190.429 185.631  28.492  1.00 16.04      A
C
ATOM     70  C   LEU A 130     186.090 185.081  29.834  1.00 21.19      A
C
ATOM     71  O   LEU A 130     186.080 183.885  30.121  1.00 24.25      A
O
ATOM     72  N   GLU A 131     185.756 186.032  30.705  1.00 23.78      A
N
ATOM     73  CA  GLU A 131     185.349 185.729  32.082  1.00 25.83      A
C
ATOM     74  CB  GLU A 131     184.952 187.016  32.834  1.00 30.42      A
C
ATOM     75  CG  GLU A 131     186.005 188.110  32.945  1.00 42.06      A
C
ATOM     76  CD  GLU A 131     186.135 188.977  31.686  1.00 46.89      A
C
ATOM     77  OE1 GLU A 131     185.319 188.822  30.747  1.00 51.89      A
O
ATOM     78  OE2 GLU A 131     187.058 189.821  31.640  1.00 50.51      A
O
ATOM     79  C   GLU A 131     184.146 184.751  32.145  1.00 25.30      A
C
ATOM     80  O   GLU A 131     183.790 184.281  33.227  1.00 21.67      A
O
ATOM     81  N   ASP A 132     183.503 184.473  31.008  1.00 22.51      A
N
ATOM     82  CA  ASP A 132     182.364 183.565  30.989  1.00 22.54      A
C
ATOM     83  CB  ASP A 132     181.458 183.825  29.782  1.00 24.79      A
C
ATOM     84  CG  ASP A 132     180.631 185.120  29.908  1.00 28.99      A
C
ATOM     85  OD1 ASP A 132     180.136 185.417  31.025  1.00 29.67      A
O
ATOM     86  OD2 ASP A 132     180.450 185.824  28.873  1.00 26.45      A
O
ATOM     87  C   ASP A 132     182.752 182.087  30.966  1.00 21.99      A
C
ATOM     88  O   ASP A 132     181.925 181.226  31.267  1.00 22.12      A
O
ATOM     89  N   PHE A 133     183.998 181.781  30.625  1.00 23.02      A
N
ATOM     90  CA  PHE A 133     184.411 180.378  30.554  1.00 22.89      A
C
ATOM     91  CB  PHE A 133     184.812 179.998  29.111  1.00 18.64      A
C
ATOM     92  CG  PHE A 133     183.901 180.565  28.039  1.00 17.41      A
C
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ATOM     93  CD1 PHE A 133     184.042 181.884  27.616  1.00 15.80      A
C
ATOM     94  CD2 PHE A 133     182.904 179.783  27.456  1.00 16.46      A
C
ATOM     95  CE1 PHE A 133     183.215 182.414  26.637  1.00 14.66      A
C
ATOM     96  CE2 PHE A 133     182.063 180.305  26.466  1.00 15.10      A
C
ATOM     97  CZ  PHE A 133     182.224 181.626  26.060  1.00 18.42      A
C
ATOM     98  C   PHE A 133     185.557 179.984  31.484  1.00 22.91      A
C
ATOM     99  O   PHE A 133     186.466 180.766  31.755  1.00 24.66      A
O
ATOM    100  N   GLU A 134     185.484 178.767  32.005  1.00 22.49      A
N
ATOM    101  CA  GLU A 134     186.566 178.248  32.814  1.00 21.74      A
C
ATOM    102  CB  GLU A 134     186.054 177.264  33.870  1.00 23.93      A
C
ATOM    103  CG  GLU A 134     185.401 177.912  35.088  1.00 29.62      A
C
ATOM    104  CD  GLU A 134     184.751 176.887  36.020  1.00 37.53      A
C
ATOM    105  OE1 GLU A 134     185.460 175.983  36.533  1.00 38.84      A
O
ATOM    106  OE2 GLU A 134     183.517 176.974  36.236  1.00 43.58      A
O
ATOM    107  C   GLU A 134     187.313 177.528  31.695  1.00 21.49      A
C
ATOM    108  O   GLU A 134     186.702 176.784  30.922  1.00 23.43      A
O
ATOM    109  N   ILE A 135     188.608 177.794  31.564  1.00 19.74      A
N
ATOM    110  CA  ILE A 135     189.425 177.197  30.524  1.00 19.08      A
C
ATOM    111  CB  ILE A 135     190.554 178.149  30.072  1.00 22.58      A
C
ATOM    112  CG2 ILE A 135     191.285 177.543  28.866  1.00 19.44      A
C
ATOM    113  CG1 ILE A 135     189.990 179.541  29.762  1.00 20.52      A
C
ATOM    114  CD1 ILE A 135     188.876 179.535  28.771  1.00 21.85      A
C
ATOM    115  C   ILE A 135     190.099 175.941  31.044  1.00 20.74      A
C
ATOM    116  O   ILE A 135     190.667 175.944  32.140  1.00 19.34      A
O
ATOM    117  N   GLY A 136     190.058 174.876  30.245  1.00 19.98      A
N
ATOM    118  CA  GLY A 136     190.688 173.629  30.637  1.00 19.38      A
C
ATOM    119  C   GLY A 136     191.995 173.397  29.906  1.00 18.61      A
C
ATOM    120  O   GLY A 136     192.742 174.324  29.668  1.00 20.61      A
O
ATOM    121  N   ARG A 137     192.267 172.156  29.533  1.00 22.50      A
N
ATOM    122  CA  ARG A 137     193.500 171.827  28.833  1.00 22.75      A
C
ATOM    123  CB  ARG A 137     193.771 170.325  28.920  1.00 22.49      A
C
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ATOM 124 CG ARG A 137 192.820 169.474 28.047 1.00 20.82 A C
ATOM 125 CD ARG A 137 193.107 168.016 28.252 1.00 15.70 A C
ATOM 126 NE ARG A 137 192.212 167.104 27.554 1.00 14.70 A N
ATOM 127 CZ ARG A 137 192.299 166.784 26.266 1.00 14.90 A C
ATOM 128 NH1 ARG A 137 193.237 167.305 25.493 1.00 13.75 A N
ATOM 129 NH2 ARG A 137 191.462 165.900 25.758 1.00 13.41 A N
ATOM 130 C ARG A 137 193.396 172.183 27.357 1.00 23.53 A C
ATOM 131 O ARG A 137 192.316 172.425 26.840 1.00 24.10 A O
ATOM 132 N PRO A 138 194.542 172.250 26.671 1.00 22.98 A N
ATOM 133 CD PRO A 138 195.850 172.477 27.313 1.00 19.97 A C
ATOM 134 CA PRO A 138 194.613 172.552 25.237 1.00 22.67 A C
ATOM 135 CB PRO A 138 196.116 172.791 25.007 1.00 21.39 A C
ATOM 136 CG PRO A 138 196.570 173.354 26.295 1.00 19.67 A C
ATOM 137 C PRO A 138 194.135 171.275 24.497 1.00 23.48 A C
ATOM 138 O PRO A 138 194.528 170.147 24.876 1.00 21.67 A O
ATOM 139 N LEU A 139 193.297 171.435 23.471 1.00 19.70 A N
ATOM 140 CA LEU A 139 192.809 170.281 22.716 1.00 19.33 A C
ATOM 141 CB LEU A 139 191.340 170.454 22.318 1.00 19.32 A C
ATOM 142 CG LEU A 139 190.349 170.509 23.473 1.00 18.46 A C
ATOM 143 CD1 LEU A 139 188.966 170.866 22.964 1.00 16.26 A C
ATOM 144 CD2 LEU A 139 190.342 169.178 24.163 1.00 15.61 A C
ATOM 145 C LEU A 139 193.636 170.125 21.454 1.00 18.97 A C
ATOM 146 O LEU A 139 193.714 169.045 20.883 1.00 20.68 A O
ATOM 147 N GLY A 140 194.256 171.215 21.026 1.00 19.57 A N
ATOM 148 CA GLY A 140 195.056 171.181 19.825 1.00 16.45 A C
ATOM 149 C GLY A 140 195.821 172.461 19.630 1.00 18.41 A C
ATOM 150 O GLY A 140 195.560 173.469 20.280 1.00 17.66 A O
ATOM 151 N LYS A 141 196.778 172.413 18.713 1.00 23.54 A N
ATOM 152 CA LYS A 141 197.635 173.547 18.399 1.00 25.64 A C
ATOM 153 CB LYS A 141 199.103 173.104 18.473 1.00 29.50 A C
ATOM 154 CG LYS A 141 200.101 174.192 18.080 1.00 37.58 A C

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ATOM    155  CD  LYS A 141     201.550 173.744  18.187  1.00 42.29      A
C
ATOM    156  CE  LYS A 141     202.483 174.918  17.891  1.00 46.12      A
C
ATOM    157  NZ  LYS A 141     203.914 174.481  17.890  1.00 49.84      A
N
ATOM    158  C   LYS A 141     197.313 174.071  16.995  1.00 26.94      A
C
ATOM    159  O   LYS A 141     197.578 173.409  15.986  1.00 26.47      A
O
ATOM    160  N   GLY A 142     196.724 175.256  16.938  1.00 26.51      A
N
ATOM    161  CA  GLY A 142     196.392 175.839  15.656  1.00 26.65      A
C
ATOM    162  C   GLY A 142     197.515 176.753  15.234  1.00 26.71      A
C
ATOM    163  O   GLY A 142     198.384 177.086  16.052  1.00 26.93      A
O
ATOM    164  N   LYS A 143     197.501 177.158  13.969  1.00 24.67      A
N
ATOM    165  CA  LYS A 143     198.529 178.037  13.452  1.00 22.25      A
C
ATOM    166  CB  LYS A 143     198.362 178.220  11.925  1.00 25.89      A
C
ATOM    167  CG  LYS A 143     199.535 178.982  11.307  1.00 30.09      A
C
ATOM    168  CD  LYS A 143     199.516 179.060   9.792  1.00 35.88      A
C
ATOM    169  CE  LYS A 143     200.619 180.037   9.330  1.00 41.66      A
C
ATOM    170  NZ  LYS A 143     200.871 180.206   7.857  1.00 42.97      A
N
ATOM    171  C   LYS A 143     198.554 179.404  14.160  1.00 22.22      A
C
ATOM    172  O   LYS A 143     199.641 179.921  14.425  1.00 22.44      A
O
ATOM    173  N   PHE A 144     197.394 179.986  14.477  1.00 20.35      A
N
ATOM    174  CA  PHE A 144     197.370 181.311  15.130  1.00 21.42      A
C
ATOM    175  CB  PHE A 144     196.429 182.258  14.362  1.00 17.68      A
C
ATOM    176  CG  PHE A 144     196.798 182.429  12.896  1.00 22.16      A
C
ATOM    177  CD1 PHE A 144     196.541 181.421  11.959  1.00 20.33      A
C
ATOM    178  CD2 PHE A 144     197.460 183.574  12.464  1.00 23.47      A
C
ATOM    179  CE1 PHE A 144     196.944 181.564  10.624  1.00 20.91      A
C
ATOM    180  CE2 PHE A 144     197.864 183.716  11.128  1.00 21.10      A
C
ATOM    181  CZ  PHE A 144     197.606 182.708  10.213  1.00 18.55      A
C
ATOM    182  C   PHE A 144     197.001 181.263  16.626  1.00 20.47      A
C
ATOM    183  O   PHE A 144     196.668 182.283  17.246  1.00 20.98      A
O
ATOM    184  N   GLY A 145     197.094 180.072  17.208  1.00 18.58      A
N
ATOM    185  CA  GLY A 145     196.786 179.915  18.616  1.00 19.23      A
C
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ATOM	186	C	GLY	A	145	196.229	178.538	18.922	1.00	20.99	A
C											
ATOM	187	O	GLY	A	145	195.911	177.756	18.016	1.00	21.28	A
O											
ATOM	188	N	ASN	A	146	196.100	178.233	20.204	1.00	20.66	A
N											
ATOM	189	CA	ASN	A	146	195.574	176.938	20.598	1.00	21.26	A
C											
ATOM	190	CB	ASN	A	146	196.140	176.544	21.964	1.00	24.59	A
C											
ATOM	191	CG	ASN	A	146	197.638	176.352	21.939	1.00	27.16	A
C											
ATOM	192	OD1	ASN	A	146	198.205	175.853	20.956	1.00	32.36	A
O											
ATOM	193	ND2	ASN	A	146	198.292	176.737	23.015	1.00	27.51	A
N											
ATOM	194	C	ASN	A	146	194.056	176.878	20.683	1.00	20.53	A
C											
ATOM	195	O	ASN	A	146	193.370	177.902	20.676	1.00	20.90	A
O											
ATOM	196	N	VAL	A	147	193.540	175.658	20.740	1.00	18.03	A
N											
ATOM	197	CA	VAL	A	147	192.121	175.430	20.922	1.00	14.64	A
C											
ATOM	198	CB	VAL	A	147	191.528	174.515	19.799	1.00	13.96	A
C											
ATOM	199	CG1	VAL	A	147	190.053	174.217	20.092	1.00	10.05	A
C											
ATOM	200	CG2	VAL	A	147	191.669	175.213	18.439	1.00	8.41	A
C											
ATOM	201	C	VAL	A	147	192.142	174.746	22.301	1.00	16.21	A
C											
ATOM	202	O	VAL	A	147	192.897	173.783	22.523	1.00	14.13	A
O											
ATOM	203	N	TYR	A	148	191.375	175.299	23.242	1.00	14.89	A
N											
ATOM	204	CA	TYR	A	148	191.315	174.786	24.614	1.00	14.47	A
C											
ATOM	205	CB	TYR	A	148	191.593	175.891	25.642	1.00	12.68	A
C											
ATOM	206	CG	TYR	A	148	192.910	176.619	25.491	1.00	18.66	A
C											
ATOM	207	CD1	TYR	A	148	193.031	177.690	24.605	1.00	16.46	A
C											
ATOM	208	CE1	TYR	A	148	194.243	178.347	24.434	1.00	18.77	A
C											
ATOM	209	CD2	TYR	A	148	194.047	176.222	26.217	1.00	15.67	A
C											
ATOM	210	CE2	TYR	A	148	195.269	176.880	26.050	1.00	20.14	A
C											
ATOM	211	CZ	TYR	A	148	195.355	177.938	25.153	1.00	18.86	A
C											
ATOM	212	OH	TYR	A	148	196.555	178.569	24.934	1.00	23.63	A
O											
ATOM	213	C	TYR	A	148	189.943	174.234	24.936	1.00	13.13	A
C											
ATOM	214	O	TYR	A	148	188.942	174.674	24.386	1.00	14.07	A
O											
ATOM	215	N	LEU	A	149	189.887	173.265	25.831	1.00	11.62	A
N											
ATOM	216	CA	LEU	A	149	188.600	172.753	26.223	1.00	11.86	A
C											

ATOM	217	CB	LEU	A	149	188.787	171.466	27.003	1.00	10.50	A
C											
ATOM	218	CG	LEU	A	149	187.547	170.675	27.388	1.00	12.61	A
C											
ATOM	219	CD1	LEU	A	149	186.695	170.364	26.182	1.00	11.20	A
C											
ATOM	220	CD2	LEU	A	149	188.001	169.410	28.051	1.00	11.24	A
C											
ATOM	221	C	LEU	A	149	188.071	173.911	27.101	1.00	13.55	A
C											
ATOM	222	O	LEU	A	149	188.857	174.728	27.565	1.00	12.48	A
O											
ATOM	223	N	ALA	A	150	186.763	174.008	27.316	1.00	14.24	A
N											
ATOM	224	CA	ALA	A	150	186.227	175.102	28.120	1.00	15.20	A
C											
ATOM	225	CB	ALA	A	150	186.230	176.406	27.318	1.00	15.60	A
C											
ATOM	226	C	ALA	A	150	184.817	174.800	28.612	1.00	17.25	A
C											
ATOM	227	O	ALA	A	150	184.122	173.929	28.083	1.00	18.30	A
O											
ATOM	228	N	ARG	A	151	184.398	175.532	29.629	1.00	17.29	A
N											
ATOM	229	CA	ARG	A	151	183.091	175.334	30.215	1.00	19.70	A
C											
ATOM	230	CB	ARG	A	151	183.245	174.479	31.492	1.00	20.02	A
C											
ATOM	231	CG	ARG	A	151	181.977	174.102	32.258	1.00	26.58	A
C											
ATOM	232	CD	ARG	A	151	182.321	173.557	33.686	1.00	30.64	A
C											
ATOM	233	NE	ARG	A	151	183.235	172.405	33.673	1.00	32.15	A
N											
ATOM	234	CZ	ARG	A	151	182.900	171.151	33.348	1.00	33.18	A
C											
ATOM	235	NH1	ARG	A	151	181.644	170.851	33.004	1.00	33.09	A
N											
ATOM	236	NH2	ARG	A	151	183.831	170.190	33.362	1.00	31.48	A
N											
ATOM	237	C	ARG	A	151	182.516	176.707	30.518	1.00	20.61	A
C											
ATOM	238	O	ARG	A	151	183.158	177.560	31.163	1.00	19.62	A
O											
ATOM	239	N	GLU	A	152	181.315	176.939	30.006	1.00	21.84	A
N											
ATOM	240	CA	GLU	A	152	180.633	178.196	30.264	1.00	21.85	A
C											
ATOM	241	CB	GLU	A	152	179.401	178.298	29.377	1.00	26.06	A
C											
ATOM	242	CG	GLU	A	152	178.766	179.690	29.289	1.00	28.31	A
C											
ATOM	243	CD	GLU	A	152	177.996	180.078	30.543	1.00	32.60	A
C											
ATOM	244	OE1	GLU	A	152	178.576	180.804	31.391	1.00	33.50	A
O											
ATOM	245	OE2	GLU	A	152	176.821	179.650	30.679	1.00	29.24	A
O											
ATOM	246	C	GLU	A	152	180.252	178.091	31.742	1.00	21.10	A
C											
ATOM	247	O	GLU	A	152	179.661	177.102	32.172	1.00	19.62	A
O											

ATOM	248	N	LYS	A	153	180.613	179.114	32.504	1.00 21.06	A
N										
ATOM	249	CA	LYS	A	153	180.366	179.156	33.933	1.00 20.90	A
C										
ATOM	250	CB	LYS	A	153	180.996	180.417	34.513	1.00 20.37	A
C										
ATOM	251	CG	LYS	A	153	182.501	180.458	34.440	1.00 22.17	A
C										
ATOM	252	CD	LYS	A	153	183.063	181.720	35.091	1.00 21.22	A
C										
ATOM	253	CE	LYS	A	153	184.568	181.658	35.002	1.00 22.77	A
C										
ATOM	254	NZ	LYS	A	153	185.178	182.877	35.572	1.00 24.11	A
N										
ATOM	255	C	LYS	A	153	178.927	179.048	34.421	1.00 21.26	A
C										
ATOM	256	O	LYS	A	153	178.649	178.362	35.390	1.00 25.58	A
O										
ATOM	257	N	GLN	A	154	177.982	179.704	33.786	1.00 23.03	A
N										
ATOM	258	CA	GLN	A	154	176.639	179.579	34.330	1.00 23.96	A
C										
ATOM	259	CB	GLN	A	154	175.744	180.686	33.800	1.00 23.79	A
C										
ATOM	260	CG	GLN	A	154	176.125	182.053	34.288	1.00 24.55	A
C										
ATOM	261	CD	GLN	A	154	175.243	183.133	33.709	1.00 24.55	A
C										
ATOM	262	OE1	GLN	A	154	175.674	184.283	33.617	1.00 23.87	A
O										
ATOM	263	NE2	GLN	A	154	173.998	182.779	33.309	1.00 22.50	A
N										
ATOM	264	C	GLN	A	154	175.951	178.229	34.086	1.00 24.10	A
C										
ATOM	265	O	GLN	A	154	175.345	177.675	34.996	1.00 25.34	A
O										
ATOM	266	N	SER	A	155	176.018	177.700	32.871	1.00 22.36	A
N										
ATOM	267	CA	SER	A	155	175.351	176.441	32.585	1.00 21.24	A
C										
ATOM	268	CB	SER	A	155	174.790	176.517	31.180	1.00 20.38	A
C										
ATOM	269	OG	SER	A	155	175.875	176.607	30.282	1.00 22.24	A
O										
ATOM	270	C	SER	A	155	176.234	175.182	32.691	1.00 23.66	A
C										
ATOM	271	O	SER	A	155	175.725	174.048	32.677	1.00 20.04	A
O										
ATOM	272	N	LYS	A	156	177.549	175.406	32.789	1.00 23.61	A
N										
ATOM	273	CA	LYS	A	156	178.572	174.358	32.849	1.00 24.47	A
C										
ATOM	274	CB	LYS	A	156	178.350	173.467	34.065	1.00 25.24	A
C										
ATOM	275	CG	LYS	A	156	178.523	174.254	35.368	1.00 32.64	A
C										
ATOM	276	CD	LYS	A	156	178.309	173.358	36.552	1.00 35.73	A
C										
ATOM	277	CE	LYS	A	156	178.506	174.079	37.870	1.00 41.50	A
C										
ATOM	278	NZ	LYS	A	156	178.457	173.059	38.978	1.00 42.75	A
N										

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ATOM    279  C   LYS A 156     178.634 173.543  31.548  1.00 22.03      A
C
ATOM    280  O   LYS A 156     179.131 172.417  31.509  1.00 22.31      A
O
ATOM    281  N   PHE A 157     178.152 174.152  30.472  1.00 20.94      A
N
ATOM    282  CA  PHE A 157     178.180 173.530  29.162  1.00 19.88      A
C
ATOM    283  CB  PHE A 157     177.370 174.367  28.174  1.00 21.87      A
C
ATOM    284  CG  PHE A 157     177.209 173.735  26.840  1.00 22.62      A
C
ATOM    285  CD1 PHE A 157     176.501 172.546  26.704  1.00 26.84      A
C
ATOM    286  CD2 PHE A 157     177.745 174.336  25.707  1.00 24.18      A
C
ATOM    287  CE1 PHE A 157     176.326 171.957  25.448  1.00 27.13      A
C
ATOM    288  CE2 PHE A 157     177.576 173.763  24.446  1.00 24.84      A
C
ATOM    289  CZ  PHE A 157     176.868 172.574  24.316  1.00 26.19      A
C
ATOM    290  C   PHE A 157     179.645 173.447  28.708  1.00 20.86      A
C
ATOM    291  O   PHE A 157     180.394 174.451  28.739  1.00 16.68      A
O
ATOM    292  N   ILE A 158     180.056 172.243  28.316  1.00 18.62      A
N
ATOM    293  CA  ILE A 158     181.412 171.997  27.862  1.00 17.65      A
C
ATOM    294  CB  ILE A 158     181.818 170.521  28.156  1.00 21.22      A
C
ATOM    295  CG2 ILE A 158     183.120 170.183  27.472  1.00 20.54      A
C
ATOM    296  CG1 ILE A 158     181.998 170.339  29.675  1.00 25.44      A
C
ATOM    297  CD1 ILE A 158     181.751 168.898  30.193  1.00 32.22      A
C
ATOM    298  C   ILE A 158     181.502 172.306  26.363  1.00 19.32      A
C
ATOM    299  O   ILE A 158     180.622 171.940  25.588  1.00 21.25      A
O
ATOM    300  N   LEU A 159     182.544 173.021  25.958  1.00 19.68      A
N
ATOM    301  CA  LEU A 159     182.729 173.365  24.552  1.00 18.03      A
C
ATOM    302  CB  LEU A 159     181.915 174.625  24.214  1.00 18.70      A
C
ATOM    303  CG  LEU A 159     181.855 175.726  25.275  1.00 18.81      A
C
ATOM    304  CD1 LEU A 159     183.137 176.522  25.197  1.00 25.89      A
C
ATOM    305  CD2 LEU A 159     180.667 176.644  25.065  1.00 15.33      A
C
ATOM    306  C   LEU A 159     184.218 173.553  24.263  1.00 16.64      A
C
ATOM    307  O   LEU A 159     185.054 173.211  25.099  1.00 10.64      A
O
ATOM    308  N   ALA A 160     184.562 174.069  23.084  1.00 14.09      A
N
ATOM    309  CA  ALA A 160     185.981 174.271  22.742  1.00 14.90      A
C
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ATOM    310  CB  ALA A 160     186.371 173.394  21.574  1.00 11.94           A
C
ATOM    311  C   ALA A 160     186.230 175.736  22.420  1.00 15.35           A
C
ATOM    312  O   ALA A 160     185.419 176.377  21.777  1.00 16.22           A
O
ATOM    313  N   LEU A 161     187.348 176.277  22.876  1.00 17.51           A
N
ATOM    314  CA  LEU A 161     187.656 177.685  22.636  1.00 17.81           A
C
ATOM    315  CB  LEU A 161     187.959 178.379  23.958  1.00 19.09           A
C
ATOM    316  CG  LEU A 161     187.661 179.882  24.003  1.00 24.28           A
C
ATOM    317  CD1 LEU A 161     186.190 180.085  23.715  1.00 19.74           A
C
ATOM    318  CD2 LEU A 161     188.020 180.482  25.396  1.00 26.64           A
C
ATOM    319  C   LEU A 161     188.857 177.829  21.697  1.00 18.94           A
C
ATOM    320  O   LEU A 161     189.984 177.506  22.070  1.00 15.15           A
O
ATOM    321  N   LYS A 162     188.605 178.302  20.477  1.00 15.44           A
N
ATOM    322  CA  LYS A 162     189.671 178.489  19.506  1.00 16.27           A
C
ATOM    323  CB  LYS A 162     189.142 178.254  18.093  1.00 15.06           A
C
ATOM    324  CG  LYS A 162     190.184 178.338  17.036  1.00 13.12           A
C
ATOM    325  CD  LYS A 162     189.615 177.968  15.682  1.00 15.23           A
C
ATOM    326  CE  LYS A 162     190.694 178.025  14.590  1.00 15.94           A
C
ATOM    327  NZ  LYS A 162     190.118 177.625  13.262  1.00 21.75           A
N
ATOM    328  C   LYS A 162     190.220 179.909  19.626  1.00 16.04           A
C
ATOM    329  O   LYS A 162     189.486 180.863  19.427  1.00 17.16           A
O
ATOM    330  N   VAL A 163     191.501 180.044  19.955  1.00 15.21           A
N
ATOM    331  CA  VAL A 163     192.110 181.357  20.107  1.00 16.50           A
C
ATOM    332  CB  VAL A 163     193.047 181.400  21.336  1.00 17.79           A
C
ATOM    333  CG1 VAL A 163     193.563 182.816  21.546  1.00 15.20           A
C
ATOM    334  CG2 VAL A 163     192.316 180.897  22.578  1.00 14.92           A
C
ATOM    335  C   VAL A 163     192.938 181.758  18.888  1.00 17.82           A
C
ATOM    336  O   VAL A 163     193.616 180.933  18.287  1.00 20.09           A
O
ATOM    337  N   LEU A 164     192.888 183.028  18.522  1.00 18.13           A
N
ATOM    338  CA  LEU A 164     193.670 183.509  17.387  1.00 15.87           A
C
ATOM    339  CB  LEU A 164     192.747 183.802  16.203  1.00 18.86           A
C
ATOM    340  CG  LEU A 164     191.903 182.603  15.752  1.00 20.75           A
C
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ATOM    341  CD1 LEU A 164     190.429 182.980  15.575  1.00 23.26      A
C
ATOM    342  CD2 LEU A 164     192.481 182.084  14.477  1.00 19.09      A
C
ATOM    343  C   LEU A 164     194.352 184.789  17.835  1.00 16.04      A
C
ATOM    344  O   LEU A 164     193.687 185.709  18.295  1.00 13.41      A
O
ATOM    345  N   PHE A 165     195.670 184.858  17.738  1.00 15.52      A
N
ATOM    346  CA  PHE A 165     196.340 186.082  18.141  1.00 18.33      A
C
ATOM    347  CB  PHE A 165     197.804 185.823  18.497  1.00 19.71      A
C
ATOM    348  CG  PHE A 165     197.987 185.214  19.850  1.00 26.23      A
C
ATOM    349  CD1 PHE A 165     197.826 183.840  20.033  1.00 27.06      A
C
ATOM    350  CD2 PHE A 165     198.222 186.025  20.961  1.00 28.47      A
C
ATOM    351  CE1 PHE A 165     197.899 183.281  21.298  1.00 32.07      A
C
ATOM    352  CE2 PHE A 165     198.299 185.479  22.239  1.00 31.56      A
C
ATOM    353  CZ  PHE A 165     198.133 184.104  22.411  1.00 35.02      A
C
ATOM    354  C   PHE A 165     196.228 187.062  16.989  1.00 19.49      A
C
ATOM    355  O   PHE A 165     196.610 186.742  15.857  1.00 21.60      A
O
ATOM    356  N   LYS A 166     195.674 188.242  17.277  1.00 18.17      A
N
ATOM    357  CA  LYS A 166     195.458 189.299  16.282  1.00 17.63      A
C
ATOM    358  CB  LYS A 166     194.786 190.520  16.931  1.00 16.68      A
C
ATOM    359  CG  LYS A 166     193.319 190.346  17.376  1.00 15.54      A
C
ATOM    360  CD  LYS A 166     192.703 191.672  17.826  1.00 10.39      A
C
ATOM    361  CE  LYS A 166     191.259 191.452  18.272  1.00 12.43      A
C
ATOM    362  NZ  LYS A 166     190.505 192.644  18.792  1.00  7.46      A
N
ATOM    363  C   LYS A 166     196.696 189.792  15.536  1.00 19.44      A
C
ATOM    364  O   LYS A 166     196.615 190.103  14.343  1.00 19.53      A
O
ATOM    365  N   ALA A 167     197.828 189.885  16.237  1.00 19.10      A
N
ATOM    366  CA  ALA A 167     199.068 190.369  15.628  1.00 18.82      A
C
ATOM    367  CB  ALA A 167     200.140 190.591  16.710  1.00 11.48      A
C
ATOM    368  C   ALA A 167     199.551 189.377  14.571  1.00 18.71      A
C
ATOM    369  O   ALA A 167     200.085 189.762  13.534  1.00 19.61      A
O
ATOM    370  N   GLN A 168     199.351 188.092  14.840  1.00 18.71      A
N
ATOM    371  CA  GLN A 168     199.734 187.039  13.907  1.00 18.86      A
C
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ATOM	372	CB	GLN	A	168	199.584	185.666	14.561	1.00	21.65	A
C											
ATOM	373	CG	GLN	A	168	200.584	184.664	14.014	1.00	25.64	A
C											
ATOM	374	CD	GLN	A	168	200.544	183.310	14.690	1.00	29.19	A
C											
ATOM	375	OE1	GLN	A	168	200.269	183.208	15.900	1.00	27.17	A
O											
ATOM	376	NE2	GLN	A	168	200.846	182.249	13.920	1.00	28.74	A
N											
ATOM	377	C	GLN	A	168	198.824	187.137	12.688	1.00	17.82	A
C											
ATOM	378	O	GLN	A	168	199.273	187.079	11.560	1.00	20.56	A
O											
ATOM	379	N	LEU	A	169	197.530	187.289	12.931	1.00	19.46	A
N											
ATOM	380	CA	LEU	A	169	196.553	187.404	11.848	1.00	19.86	A
C											
ATOM	381	CB	LEU	A	169	195.146	187.572	12.393	1.00	20.65	A
C											
ATOM	382	CG	LEU	A	169	194.514	186.370	13.052	1.00	24.58	A
C											
ATOM	383	CD1	LEU	A	169	193.168	186.837	13.566	1.00	23.53	A
C											
ATOM	384	CD2	LEU	A	169	194.396	185.189	12.069	1.00	20.67	A
C											
ATOM	385	C	LEU	A	169	196.802	188.604	10.961	1.00	21.12	A
C											
ATOM	386	O	LEU	A	169	196.533	188.564	9.761	1.00	17.39	A
O											
ATOM	387	N	GLU	A	170	197.261	189.697	11.564	1.00	22.51	A
N											
ATOM	388	CA	GLU	A	170	197.520	190.915	10.807	1.00	23.02	A
C											
ATOM	389	CB	GLU	A	170	197.637	192.102	11.769	1.00	22.68	A
C											
ATOM	390	CG	GLU	A	170	196.267	192.607	12.232	1.00	27.99	A
C											
ATOM	391	CD	GLU	A	170	196.294	193.330	13.579	1.00	31.84	A
C											
ATOM	392	OE1	GLU	A	170	197.334	193.955	13.920	1.00	33.33	A
O											
ATOM	393	OE2	GLU	A	170	195.256	193.278	14.285	1.00	31.22	A
O											
ATOM	394	C	GLU	A	170	198.762	190.753	9.949	1.00	21.03	A
C											
ATOM	395	O	GLU	A	170	198.739	191.068	8.757	1.00	23.09	A
O											
ATOM	396	N	LYS	A	171	199.826	190.220	10.535	1.00	17.25	A
N											
ATOM	397	CA	LYS	A	171	201.059	190.014	9.790	1.00	19.63	A
C											
ATOM	398	CB	LYS	A	171	202.139	189.442	10.706	1.00	21.18	A
C											
ATOM	399	CG	LYS	A	171	203.525	189.395	10.073	1.00	25.15	A
C											
ATOM	400	CD	LYS	A	171	204.574	188.888	11.054	1.00	28.24	A
C											
ATOM	401	CE	LYS	A	171	205.952	188.807	10.395	1.00	32.60	A
C											
ATOM	402	NZ	LYS	A	171	207.003	188.297	11.331	1.00	33.23	A
N											

ATOM	403	C	LYS	A	171	200.838	189.074	8.609	1.00	19.42	A
C											
ATOM	404	O	LYS	A	171	201.451	189.235	7.551	1.00	21.92	A
O											
ATOM	405	N	ALA	A	172	199.957	188.095	8.782	1.00	17.92	A
N											
ATOM	406	CA	ALA	A	172	199.666	187.126	7.720	1.00	18.61	A
C											
ATOM	407	CB	ALA	A	172	199.168	185.826	8.341	1.00	13.39	A
C											
ATOM	408	C	ALA	A	172	198.666	187.627	6.679	1.00	16.48	A
C											
ATOM	409	O	ALA	A	172	198.600	187.082	5.577	1.00	18.45	A
O											
ATOM	410	N	GLY	A	173	197.890	188.651	7.053	1.00	16.48	A
N											
ATOM	411	CA	GLY	A	173	196.876	189.241	6.178	1.00	17.37	A
C											
ATOM	412	C	GLY	A	173	195.719	188.297	5.904	1.00	18.48	A
C											
ATOM	413	O	GLY	A	173	195.158	188.264	4.789	1.00	17.50	A
O											
ATOM	414	N	VAL	A	174	195.344	187.536	6.921	1.00	16.39	A
N											
ATOM	415	CA	VAL	A	174	194.274	186.573	6.770	1.00	18.80	A
C											
ATOM	416	CB	VAL	A	174	194.778	185.171	7.226	1.00	17.75	A
C											
ATOM	417	CG1	VAL	A	174	195.976	184.770	6.371	1.00	17.03	A
C											
ATOM	418	CG2	VAL	A	174	195.166	185.207	8.684	1.00	12.69	A
C											
ATOM	419	C	VAL	A	174	193.015	186.982	7.535	1.00	19.69	A
C											
ATOM	420	O	VAL	A	174	192.152	186.152	7.828	1.00	22.14	A
O											
ATOM	421	N	GLU	A	175	192.900	188.282	7.801	1.00	24.29	A
N											
ATOM	422	CA	GLU	A	175	191.751	188.834	8.521	1.00	25.76	A
C											
ATOM	423	CB	GLU	A	175	191.902	190.351	8.799	1.00	29.22	A
C											
ATOM	424	CG	GLU	A	175	193.333	190.938	8.903	1.00	38.41	A
C											
ATOM	425	CD	GLU	A	175	193.998	191.112	7.548	1.00	39.97	A
C											
ATOM	426	OE1	GLU	A	175	193.310	190.986	6.511	1.00	47.49	A
O											
ATOM	427	OE2	GLU	A	175	195.206	191.382	7.507	1.00	46.22	A
O											
ATOM	428	C	GLU	A	175	190.452	188.611	7.752	1.00	25.95	A
C											
ATOM	429	O	GLU	A	175	189.423	188.313	8.337	1.00	25.42	A
O											
ATOM	430	N	HIS	A	176	190.483	188.768	6.438	1.00	26.45	A
N											
ATOM	431	CA	HIS	A	176	189.254	188.539	5.708	1.00	24.68	A
C											
ATOM	432	CB	HIS	A	176	189.316	189.074	4.278	1.00	23.09	A
C											
ATOM	433	CG	HIS	A	176	187.983	189.014	3.596	1.00	32.41	A
C											

ATOM	434	CD2	HIS	A	176	187.570	188.363	2.477	1.00	34.18	A
C											
ATOM	435	ND1	HIS	A	176	186.845	189.576	4.148	1.00	32.75	A
N											
ATOM	436	CE1	HIS	A	176	185.796	189.266	3.406	1.00	33.74	A
C											
ATOM	437	NE2	HIS	A	176	186.207	188.529	2.386	1.00	34.72	A
N											
ATOM	438	C	HIS	A	176	188.848	187.062	5.703	1.00	23.32	A
C											
ATOM	439	O	HIS	A	176	187.661	186.755	5.693	1.00	22.64	A
O											
ATOM	440	N	GLN	A	177	189.803	186.137	5.744	1.00	21.78	A
N											
ATOM	441	CA	GLN	A	177	189.432	184.721	5.774	1.00	19.85	A
C											
ATOM	442	CB	GLN	A	177	190.628	183.818	5.421	1.00	21.23	A
C											
ATOM	443	CG	GLN	A	177	191.173	183.994	3.977	1.00	23.08	A
C											
ATOM	444	CD	GLN	A	177	192.113	185.179	3.856	1.00	26.14	A
C											
ATOM	445	OE1	GLN	A	177	191.901	186.204	4.512	1.00	27.02	A
O											
ATOM	446	NE2	GLN	A	177	193.161	185.056	3.012	1.00	25.09	A
N											
ATOM	447	C	GLN	A	177	188.859	184.317	7.129	1.00	18.66	A
C											
ATOM	448	O	GLN	A	177	188.057	183.390	7.195	1.00	18.16	A
O											
ATOM	449	N	LEU	A	178	189.267	185.001	8.202	1.00	17.80	A
N											
ATOM	450	CA	LEU	A	178	188.742	184.695	9.532	1.00	17.25	A
C											
ATOM	451	CB	LEU	A	178	189.473	185.495	10.616	1.00	14.48	A
C											
ATOM	452	CG	LEU	A	178	188.948	185.297	12.041	1.00	14.78	A
C											
ATOM	453	CD1	LEU	A	178	188.822	183.792	12.391	1.00	13.65	A
C											
ATOM	454	CD2	LEU	A	178	189.904	185.964	13.002	1.00	15.52	A
C											
ATOM	455	C	LEU	A	178	187.257	185.050	9.569	1.00	18.82	A
C											
ATOM	456	O	LEU	A	178	186.436	184.346	10.148	1.00	18.56	A
O											
ATOM	457	N	ARG	A	179	186.929	186.171	8.950	1.00	17.14	A
N											
ATOM	458	CA	ARG	A	179	185.570	186.637	8.893	1.00	20.36	A
C											
ATOM	459	CB	ARG	A	179	185.547	188.004	8.238	1.00	24.60	A
C											
ATOM	460	CG	ARG	A	179	184.191	188.581	8.190	1.00	30.51	A
C											
ATOM	461	CD	ARG	A	179	184.079	189.355	6.937	1.00	34.92	A
C											
ATOM	462	NE	ARG	A	179	183.602	190.700	7.192	1.00	44.42	A
N											
ATOM	463	CZ	ARG	A	179	184.338	191.679	7.721	1.00	50.64	A
C											
ATOM	464	NH1	ARG	A	179	185.609	191.475	8.060	1.00	53.62	A
N											

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ATOM    465  NH2 ARG A 179     183.800 192.881   7.910  1.00 54.27      A
N
ATOM    466  C   ARG A 179     184.677 185.663   8.112  1.00 20.68      A
C
ATOM    467  O   ARG A 179     183.516 185.428   8.490  1.00 20.49      A
O
ATOM    468  N   ARG A 180     185.211 185.102   7.027  1.00 16.87      A
N
ATOM    469  CA  ARG A 180     184.457 184.139   6.240  1.00 16.27      A
C
ATOM    470  CB  ARG A 180     185.145 183.851   4.880  1.00 15.64      A
C
ATOM    471  CG  ARG A 180     185.036 184.997   3.869  1.00 19.03      A
C
ATOM    472  CD  ARG A 180     185.243 184.593   2.394  1.00 19.17      A
C
ATOM    473  NE  ARG A 180     186.536 183.973   2.158  1.00 22.25      A
N
ATOM    474  CZ  ARG A 180     187.223 184.003   1.011  1.00 22.42      A
C
ATOM    475  NH1 ARG A 180     186.778 184.633  -0.067  1.00 16.67      A
N
ATOM    476  NH2 ARG A 180     188.390 183.384   0.949  1.00 23.03      A
N
ATOM    477  C   ARG A 180     184.277 182.837   7.037  1.00 16.14      A
C
ATOM    478  O   ARG A 180     183.225 182.207   6.950  1.00 17.78      A
O
ATOM    479  N   GLU A 181     185.294 182.439   7.812  1.00 15.13      A
N
ATOM    480  CA  GLU A 181     185.211 181.222   8.627  1.00 15.82      A
C
ATOM    481  CB  GLU A 181     186.512 180.969   9.431  1.00 17.60      A
C
ATOM    482  CG  GLU A 181     186.517 179.610  10.164  1.00 22.11      A
C
ATOM    483  CD  GLU A 181     187.779 179.293  11.023  1.00 29.50      A
C
ATOM    484  OE1 GLU A 181     188.877 179.898  10.811  1.00 23.91      A
O
ATOM    485  OE2 GLU A 181     187.654 178.393  11.914  1.00 30.52      A
O
ATOM    486  C   GLU A 181     184.059 181.374   9.615  1.00 17.24      A
C
ATOM    487  O   GLU A 181     183.169 180.514   9.711  1.00 17.81      A
O
ATOM    488  N   VAL A 182     184.075 182.486  10.336  1.00 13.24      A
N
ATOM    489  CA  VAL A 182     183.056 182.746  11.323  1.00 16.10      A
C
ATOM    490  CB  VAL A 182     183.417 183.989  12.155  1.00 17.20      A
C
ATOM    491  CG1 VAL A 182     182.271 184.362  13.059  1.00 11.33      A
C
ATOM    492  CG2 VAL A 182     184.675 183.709  12.948  1.00 15.06      A
C
ATOM    493  C   VAL A 182     181.650 182.907  10.756  1.00 16.14      A
C
ATOM    494  O   VAL A 182     180.718 182.216  11.186  1.00 14.19      A
O
ATOM    495  N   GLU A 183     181.491 183.805   9.788  1.00 16.25      A
N
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ATOM	496	CA	GLU	A	183	180.162	184.021	9.212	1.00	17.30	A
C											
ATOM	497	CB	GLU	A	183	180.190	185.187	8.214	1.00	16.51	A
C											
ATOM	498	CG	GLU	A	183	180.630	186.499	8.842	1.00	21.63	A
C											
ATOM	499	CD	GLU	A	183	180.566	187.674	7.874	1.00	24.47	A
C											
ATOM	500	OE1	GLU	A	183	180.841	187.477	6.673	1.00	27.21	A
O											
ATOM	501	OE2	GLU	A	183	180.255	188.801	8.315	1.00	29.43	A
O											
ATOM	502	C	GLU	A	183	179.581	182.764	8.555	1.00	14.99	A
C											
ATOM	503	O	GLU	A	183	178.405	182.460	8.753	1.00	16.33	A
O											
ATOM	504	N	ILE	A	184	180.396	182.019	7.810	1.00	12.00	A
N											
ATOM	505	CA	ILE	A	184	179.908	180.808	7.159	1.00	10.45	A
C											
ATOM	506	CB	ILE	A	184	180.904	180.302	6.094	1.00	9.02	A
C											
ATOM	507	CG2	ILE	A	184	180.595	178.854	5.712	1.00	2.93	A
C											
ATOM	508	CG1	ILE	A	184	180.862	181.248	4.893	1.00	4.36	A
C											
ATOM	509	CD1	ILE	A	184	182.025	181.076	3.939	1.00	5.66	A
C											
ATOM	510	C	ILE	A	184	179.633	179.675	8.149	1.00	12.74	A
C											
ATOM	511	O	ILE	A	184	178.552	179.077	8.135	1.00	13.03	A
O											
ATOM	512	N	GLN	A	185	180.585	179.380	9.026	1.00	14.41	A
N											
ATOM	513	CA	GLN	A	185	180.365	178.279	9.960	1.00	15.94	A
C											
ATOM	514	CB	GLN	A	185	181.663	177.933	10.682	1.00	15.68	A
C											
ATOM	515	CG	GLN	A	185	181.684	176.556	11.281	1.00	15.22	A
C											
ATOM	516	CD	GLN	A	185	182.955	176.333	12.074	1.00	16.62	A
C											
ATOM	517	OE1	GLN	A	185	183.844	177.184	12.072	1.00	19.84	A
O											
ATOM	518	NE2	GLN	A	185	183.048	175.198	12.760	1.00	15.50	A
N											
ATOM	519	C	GLN	A	185	179.257	178.551	10.977	1.00	14.85	A
C											
ATOM	520	O	GLN	A	185	178.507	177.637	11.339	1.00	11.63	A
O											
ATOM	521	N	SER	A	186	179.134	179.798	11.424	1.00	14.21	A
N											
ATOM	522	CA	SER	A	186	178.102	180.102	12.421	1.00	15.30	A
C											
ATOM	523	CB	SER	A	186	178.265	181.527	13.028	1.00	15.24	A
C											
ATOM	524	OG	SER	A	186	178.146	182.584	12.086	1.00	16.11	A
O											
ATOM	525	C	SER	A	186	176.686	179.916	11.898	1.00	15.48	A
C											
ATOM	526	O	SER	A	186	175.787	179.612	12.672	1.00	20.12	A
O											

ATOM	527	N	HIS	A	187	176.483	180.048	10.592	1.00	15.79	A
N											
ATOM	528	CA	HIS	A	187	175.153	179.908	10.018	1.00	15.76	A
C											
ATOM	529	CB	HIS	A	187	174.964	180.942	8.914	1.00	14.22	A
C											
ATOM	530	CG	HIS	A	187	174.857	182.348	9.414	1.00	14.55	A
C											
ATOM	531	CD2	HIS	A	187	173.787	183.070	9.816	1.00	12.55	A
C											
ATOM	532	ND1	HIS	A	187	175.944	183.189	9.516	1.00	13.11	A
N											
ATOM	533	CE1	HIS	A	187	175.548	184.369	9.951	1.00	10.14	A
C											
ATOM	534	NE2	HIS	A	187	174.243	184.324	10.140	1.00	15.06	A
N											
ATOM	535	C	HIS	A	187	174.838	178.515	9.469	1.00	17.67	A
C											
ATOM	536	O	HIS	A	187	173.762	178.272	8.931	1.00	17.40	A
O											
ATOM	537	N	LEU	A	188	175.777	177.595	9.616	1.00	18.89	A
N											
ATOM	538	CA	LEU	A	188	175.608	176.243	9.118	1.00	16.21	A
C											
ATOM	539	CB	LEU	A	188	176.972	175.721	8.652	1.00	15.40	A
C											
ATOM	540	CG	LEU	A	188	177.339	175.433	7.185	1.00	14.79	A
C											
ATOM	541	CD1	LEU	A	188	176.514	176.200	6.155	1.00	14.64	A
C											
ATOM	542	CD2	LEU	A	188	178.805	175.738	7.024	1.00	11.29	A
C											
ATOM	543	C	LEU	A	188	175.047	175.408	10.266	1.00	17.59	A
C											
ATOM	544	O	LEU	A	188	175.382	175.630	11.423	1.00	19.21	A
O											
ATOM	545	N	ARG	A	189	174.174	174.458	9.955	1.00	19.36	A
N											
ATOM	546	CA	ARG	A	189	173.579	173.603	10.988	1.00	21.36	A
C											
ATOM	547	CB	ARG	A	189	172.190	174.086	11.398	1.00	22.58	A
C											
ATOM	548	CG	ARG	A	189	172.131	175.420	12.110	1.00	32.57	A
C											
ATOM	549	CD	ARG	A	189	172.277	175.274	13.621	1.00	34.83	A
C											
ATOM	550	NE	ARG	A	189	172.168	176.568	14.298	1.00	40.56	A
N											
ATOM	551	CZ	ARG	A	189	172.993	177.598	14.091	1.00	43.35	A
C											
ATOM	552	NH1	ARG	A	189	173.993	177.481	13.215	1.00	42.31	A
N											
ATOM	553	NH2	ARG	A	189	172.827	178.740	14.770	1.00	42.32	A
N											
ATOM	554	C	ARG	A	189	173.423	172.219	10.415	1.00	19.45	A
C											
ATOM	555	O	ARG	A	189	172.582	171.996	9.558	1.00	19.37	A
O											
ATOM	556	N	HIS	A	190	174.218	171.283	10.900	1.00	16.48	A
N											
ATOM	557	CA	HIS	A	190	174.148	169.936	10.388	1.00	16.32	A
C											

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ATOM    558  CB  HIS A 190     174.865 169.868   9.042  1.00 13.06      A
C
ATOM    559  CG  HIS A 190     174.848 168.517   8.403  1.00  8.96      A
C
ATOM    560  CD2 HIS A 190     175.640 167.430   8.584  1.00  9.19      A
C
ATOM    561  ND1 HIS A 190     173.942 168.169   7.422  1.00  9.60      A
N
ATOM    562  CE1 HIS A 190     174.177 166.929   7.026  1.00  8.25      A
C
ATOM    563  NE2 HIS A 190     175.202 166.456   7.717  1.00 10.48      A
N
ATOM    564  C   HIS A 190     174.857 169.069  11.409  1.00 18.77      A
C
ATOM    565  O   HIS A 190     175.747 169.538  12.110  1.00 19.58      A
O
ATOM    566  N   PRO A 191     174.437 167.797  11.526  1.00 19.81      A
N
ATOM    567  CD  PRO A 191     173.236 167.329  10.808  1.00 18.67      A
C
ATOM    568  CA  PRO A 191     174.946 166.749  12.430  1.00 18.82      A
C
ATOM    569  CB  PRO A 191     174.058 165.545  12.108  1.00 15.98      A
C
ATOM    570  CG  PRO A 191     172.813 166.147  11.615  1.00 19.49      A
C
ATOM    571  C   PRO A 191     176.422 166.383  12.239  1.00 15.63      A
C
ATOM    572  O   PRO A 191     177.074 165.908  13.167  1.00 16.18      A
O
ATOM    573  N   ASN A 192     176.930 166.564  11.029  1.00 13.38      A
N
ATOM    574  CA  ASN A 192     178.306 166.216  10.740  1.00 13.06      A
C
ATOM    575  CB  ASN A 192     178.367 165.242   9.568  1.00 16.94      A
C
ATOM    576  CG  ASN A 192     177.621 163.963   9.853  1.00 21.40      A
C
ATOM    577  OD1 ASN A 192     176.478 163.790   9.431  1.00 24.81      A
O
ATOM    578  ND2 ASN A 192     178.255 163.062  10.596  1.00 19.25      A
N
ATOM    579  C   ASN A 192     179.189 167.407  10.467  1.00 13.65      A
C
ATOM    580  O   ASN A 192     180.258 167.276   9.869  1.00 15.58      A
O
ATOM    581  N   ILE A 193     178.725 168.584  10.865  1.00 13.34      A
N
ATOM    582  CA  ILE A 193     179.529 169.789  10.734  1.00 12.06      A
C
ATOM    583  CB  ILE A 193     178.886 170.843   9.814  1.00 11.35      A
C
ATOM    584  CG2 ILE A 193     179.688 172.131   9.882  1.00  5.81      A
C
ATOM    585  CG1 ILE A 193     178.807 170.317   8.381  1.00  6.17      A
C
ATOM    586  CD1 ILE A 193     178.045 171.205   7.453  1.00  8.69      A
C
ATOM    587  C   ILE A 193     179.651 170.377  12.134  1.00 12.85      A
C
ATOM    588  O   ILE A 193     178.663 170.540  12.840  1.00 14.90      A
O
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ATOM	589	N	LEU	A	194	180.874	170.678	12.530	1.00	13.66	A
N											
ATOM	590	CA	LEU	A	194	181.123	171.253	13.839	1.00	14.76	A
C											
ATOM	591	CB	LEU	A	194	182.623	171.519	14.036	1.00	16.68	A
C											
ATOM	592	CG	LEU	A	194	183.117	171.537	15.486	1.00	15.84	A
C											
ATOM	593	CD1	LEU	A	194	183.039	170.099	16.000	1.00	14.02	A
C											
ATOM	594	CD2	LEU	A	194	184.545	172.073	15.588	1.00	14.49	A
C											
ATOM	595	C	LEU	A	194	180.381	172.578	13.964	1.00	16.81	A
C											
ATOM	596	O	LEU	A	194	180.450	173.433	13.070	1.00	18.34	A
O											
ATOM	597	N	ARG	A	195	179.683	172.727	15.085	1.00	15.08	A
N											
ATOM	598	CA	ARG	A	195	178.924	173.924	15.390	1.00	16.45	A
C											
ATOM	599	CB	ARG	A	195	177.878	173.634	16.474	1.00	19.44	A
C											
ATOM	600	CG	ARG	A	195	176.596	172.975	15.987	1.00	25.93	A
C											
ATOM	601	CD	ARG	A	195	175.746	173.967	15.232	1.00	29.82	A
C											
ATOM	602	NE	ARG	A	195	174.811	174.694	16.091	1.00	36.41	A
N											
ATOM	603	CZ	ARG	A	195	174.859	176.008	16.302	1.00	39.91	A
C											
ATOM	604	NH1	ARG	A	195	175.804	176.729	15.718	1.00	44.61	A
N											
ATOM	605	NH2	ARG	A	195	173.958	176.608	17.075	1.00	40.14	A
N											
ATOM	606	C	ARG	A	195	179.787	175.113	15.870	1.00	16.17	A
C											
ATOM	607	O	ARG	A	195	180.714	174.950	16.656	1.00	13.03	A
O											
ATOM	608	N	LEU	A	196	179.471	176.293	15.341	1.00	17.85	A
N											
ATOM	609	CA	LEU	A	196	180.114	177.536	15.749	1.00	16.50	A
C											
ATOM	610	CB	LEU	A	196	180.623	178.380	14.572	1.00	13.17	A
C											
ATOM	611	CG	LEU	A	196	181.348	179.669	14.959	1.00	15.31	A
C											
ATOM	612	CD1	LEU	A	196	182.467	179.277	15.910	1.00	13.98	A
C											
ATOM	613	CD2	LEU	A	196	181.922	180.404	13.749	1.00	12.29	A
C											
ATOM	614	C	LEU	A	196	178.975	178.281	16.466	1.00	15.90	A
C											
ATOM	615	O	LEU	A	196	178.037	178.767	15.839	1.00	15.06	A
O											
ATOM	616	N	TYR	A	197	179.062	178.337	17.791	1.00	18.19	A
N											
ATOM	617	CA	TYR	A	197	178.049	178.974	18.610	1.00	18.38	A
C											
ATOM	618	CB	TYR	A	197	178.154	178.464	20.033	1.00	15.79	A
C											
ATOM	619	CG	TYR	A	197	177.908	176.980	20.126	1.00	17.64	A
C											

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ATOM    620  CD1 TYR A 197     178.955 176.080  20.280  1.00 15.26      A
C
ATOM    621  CE1 TYR A 197     178.712 174.718  20.364  1.00 20.64      A
C
ATOM    622  CD2 TYR A 197     176.607 176.469  20.054  1.00 21.32      A
C
ATOM    623  CE2 TYR A 197     176.360 175.104  20.138  1.00 20.23      A
C
ATOM    624  CZ  TYR A 197     177.418 174.242  20.293  1.00 20.94      A
C
ATOM    625  OH  TYR A 197     177.185 172.900  20.387  1.00 26.42      A
O
ATOM    626  C   TYR A 197     178.174 180.481  18.561  1.00 19.88      A
C
ATOM    627  O   TYR A 197     177.180 181.193  18.454  1.00 19.95      A
O
ATOM    628  N   GLY A 198     179.394 180.985  18.611  1.00 20.35      A
N
ATOM    629  CA  GLY A 198     179.542 182.425  18.562  1.00 20.00      A
C
ATOM    630  C   GLY A 198     180.984 182.838  18.642  1.00 17.90      A
C
ATOM    631  O   GLY A 198     181.874 182.005  18.677  1.00 19.17      A
O
ATOM    632  N   TYR A 199     181.222 184.134  18.686  1.00 17.72      A
N
ATOM    633  CA  TYR A 199     182.589 184.593  18.748  1.00 19.93      A
C
ATOM    634  CB  TYR A 199     183.128 184.776  17.325  1.00 19.83      A
C
ATOM    635  CG  TYR A 199     182.894 186.166  16.788  1.00 21.41      A
C
ATOM    636  CD1 TYR A 199     183.892 187.135  16.885  1.00 21.65      A
C
ATOM    637  CE1 TYR A 199     183.677 188.430  16.486  1.00 22.65      A
C
ATOM    638  CD2 TYR A 199     181.660 186.538  16.266  1.00 18.59      A
C
ATOM    639  CE2 TYR A 199     181.426 187.841  15.862  1.00 22.04      A
C
ATOM    640  CZ  TYR A 199     182.439 188.787  15.972  1.00 23.54      A
C
ATOM    641  OH  TYR A 199     182.223 190.089  15.557  1.00 24.04      A
O
ATOM    642  C   TYR A 199     182.693 185.910  19.508  1.00 19.03      A
C
ATOM    643  O   TYR A 199     181.703 186.618  19.699  1.00 19.48      A
O
ATOM    644  N   PHE A 200     183.910 186.238  19.920  1.00 18.13      A
N
ATOM    645  CA  PHE A 200     184.177 187.478  20.627  1.00 17.58      A
C
ATOM    646  CB  PHE A 200     183.677 187.397  22.091  1.00 12.35      A
C
ATOM    647  CG  PHE A 200     184.369 186.344  22.955  1.00 13.81      A
C
ATOM    648  CD1 PHE A 200     185.449 186.685  23.779  1.00 14.44      A
C
ATOM    649  CD2 PHE A 200     183.898 185.033  22.998  1.00 12.16      A
C
ATOM    650  CE1 PHE A 200     186.043 185.731  24.636  1.00 13.44      A
C
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ATOM    651  CE2 PHE A 200     184.474 184.075  23.845  1.00 13.42      A
C
ATOM    652  CZ  PHE A 200     185.552 184.426  24.669  1.00 13.28      A
C
ATOM    653  C   PHE A 200     185.675 187.756  20.549  1.00 18.86      A
C
ATOM    654  O   PHE A 200     186.482 186.840  20.451  1.00 24.13      A
O
ATOM    655  N   HIS A 201     186.056 189.019  20.573  1.00 19.06      A
N
ATOM    656  CA  HIS A 201     187.467 189.335  20.512  1.00 22.05      A
C
ATOM    657  CB  HIS A 201     187.820 189.966  19.159  1.00 20.51      A
C
ATOM    658  CG  HIS A 201     187.161 191.286  18.903  1.00 18.99      A
C
ATOM    659  CD2 HIS A 201     185.922 191.593  18.450  1.00 19.83      A
C
ATOM    660  ND1 HIS A 201     187.848 192.478  18.965  1.00 21.28      A
N
ATOM    661  CE1 HIS A 201     187.071 193.459  18.544  1.00 19.32      A
C
ATOM    662  NE2 HIS A 201     185.896 192.948  18.223  1.00 20.12      A
N
ATOM    663  C   HIS A 201     187.840 190.279  21.629  1.00 22.96      A
C
ATOM    664  O   HIS A 201     186.977 190.871  22.253  1.00 23.67      A
O
ATOM    665  N   ASP A 202     189.126 190.395  21.913  1.00 23.03      A
N
ATOM    666  CA  ASP A 202     189.535 191.331  22.936  1.00 24.25      A
C
ATOM    667  CB  ASP A 202     189.928 190.621  24.235  1.00 25.39      A
C
ATOM    668  CG  ASP A 202     191.175 189.780  24.097  1.00 28.38      A
C
ATOM    669  OD1 ASP A 202     191.836 189.826  23.031  1.00 34.60      A
O
ATOM    670  OD2 ASP A 202     191.495 189.066  25.067  1.00 24.71      A
O
ATOM    671  C   ASP A 202     190.696 192.148  22.398  1.00 25.07      A
C
ATOM    672  O   ASP A 202     190.896 192.235  21.193  1.00 24.05      A
O
ATOM    673  N   ALA A 203     191.480 192.733  23.287  1.00 26.38      A
N
ATOM    674  CA  ALA A 203     192.595 193.564  22.856  1.00 25.39      A
C
ATOM    675  CB  ALA A 203     193.217 194.257  24.082  1.00 23.30      A
C
ATOM    676  C   ALA A 203     193.678 192.847  22.039  1.00 25.31      A
C
ATOM    677  O   ALA A 203     194.184 193.405  21.070  1.00 24.76      A
O
ATOM    678  N   THR A 204     194.038 191.623  22.409  1.00 24.17      A
N
ATOM    679  CA  THR A 204     195.084 190.922  21.682  1.00 24.93      A
C
ATOM    680  CB  THR A 204     196.202 190.467  22.631  1.00 28.17      A
C
ATOM    681  OG1 THR A 204     195.667 189.534  23.582  1.00 29.58      A
O
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ATOM    682  CG2 THR A 204     196.805 191.672  23.364  1.00 26.38      A
C
ATOM    683  C   THR A 204     194.638 189.711  20.869  1.00 26.55      A
C
ATOM    684  O   THR A 204     195.360 189.270  19.968  1.00 25.70      A
O
ATOM    685  N   ARG A 205     193.469 189.149  21.166  1.00 26.89      A
N
ATOM    686  CA  ARG A 205     193.039 188.002  20.382  1.00 26.09      A
C
ATOM    687  CB  ARG A 205     193.558 186.710  21.026  1.00 29.89      A
C
ATOM    688  CG  ARG A 205     193.403 186.595  22.508  1.00 35.65      A
C
ATOM    689  CD  ARG A 205     194.768 186.465  23.174  1.00 41.67      A
C
ATOM    690  NE  ARG A 205     194.650 186.517  24.630  1.00 50.08      A
N
ATOM    691  CZ  ARG A 205     195.657 186.756  25.467  1.00 53.61      A
C
ATOM    692  NH1 ARG A 205     196.884 186.972  24.997  1.00 54.63      A
N
ATOM    693  NH2 ARG A 205     195.429 186.782  26.781  1.00 57.41      A
N
ATOM    694  C   ARG A 205     191.561 187.869  20.036  1.00 23.76      A
C
ATOM    695  O   ARG A 205     190.728 188.654  20.478  1.00 26.35      A
O
ATOM    696  N   VAL A 206     191.253 186.892  19.187  1.00 21.67      A
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ATOM    697  CA  VAL A 206     189.883 186.606  18.776  1.00 17.07      A
C
ATOM    698  CB  VAL A 206     189.704 186.683  17.247  1.00 16.64      A
C
ATOM    699  CG1 VAL A 206     188.235 186.422  16.888  1.00 11.75      A
C
ATOM    700  CG2 VAL A 206     190.136 188.055  16.741  1.00 15.29      A
C
ATOM    701  C   VAL A 206     189.541 185.179  19.225  1.00 16.35      A
C
ATOM    702  O   VAL A 206     190.380 184.277  19.146  1.00 15.34      A
O
ATOM    703  N   TYR A 207     188.308 184.987  19.688  1.00 15.70      A
N
ATOM    704  CA  TYR A 207     187.866 183.692  20.185  1.00 14.78      A
C
ATOM    705  CB  TYR A 207     187.555 183.754  21.686  1.00 14.30      A
C
ATOM    706  CG  TYR A 207     188.599 184.415  22.538  1.00 15.34      A
C
ATOM    707  CD1 TYR A 207     188.725 185.809  22.565  1.00 15.56      A
C
ATOM    708  CE1 TYR A 207     189.669 186.433  23.389  1.00 14.72      A
C
ATOM    709  CD2 TYR A 207     189.445 183.655  23.347  1.00 13.39      A
C
ATOM    710  CE2 TYR A 207     190.393 184.263  24.174  1.00 15.70      A
C
ATOM    711  CZ  TYR A 207     190.497 185.652  24.192  1.00 16.96      A
C
ATOM    712  OH  TYR A 207     191.413 186.252  25.028  1.00 17.44      A
O
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ATOM    713  C   TYR A 207     186.624 183.132  19.506  1.00 14.64      A
C
ATOM    714  O   TYR A 207     185.604 183.807  19.390  1.00 14.86      A
O
ATOM    715  N   LEU A 208     186.716 181.882  19.082  1.00 12.98      A
N
ATOM    716  CA  LEU A 208     185.597 181.206  18.475  1.00 11.35      A
C
ATOM    717  CB  LEU A 208     186.025 180.515  17.181  1.00 12.38      A
C
ATOM    718  CG  LEU A 208     186.790 181.296  16.101  1.00 18.53      A
C
ATOM    719  CD1 LEU A 208     186.415 180.695  14.759  1.00 13.01      A
C
ATOM    720  CD2 LEU A 208     186.466 182.794  16.118  1.00 17.18      A
C
ATOM    721  C   LEU A 208     185.092 180.162  19.473  1.00 11.42      A
C
ATOM    722  O   LEU A 208     185.875 179.354  19.978  1.00  9.69      A
O
ATOM    723  N   ILE A 209     183.789 180.194  19.753  1.00 11.10      A
N
ATOM    724  CA  ILE A 209     183.146 179.268  20.670  1.00 10.69      A
C
ATOM    725  CB  ILE A 209     181.968 179.962  21.389  1.00 13.97      A
C
ATOM    726  CG2 ILE A 209     181.316 178.980  22.422  1.00 10.28      A
C
ATOM    727  CG1 ILE A 209     182.489 181.303  21.979  1.00 14.77      A
C
ATOM    728  CD1 ILE A 209     181.466 182.209  22.621  1.00 10.27      A
C
ATOM    729  C   ILE A 209     182.659 178.124  19.785  1.00 13.02      A
C
ATOM    730  O   ILE A 209     181.689 178.238  19.040  1.00 13.94      A
O
ATOM    731  N   LEU A 210     183.373 177.019  19.856  1.00 12.66      A
N
ATOM    732  CA  LEU A 210     183.065 175.867  19.044  1.00 13.21      A
C
ATOM    733  CB  LEU A 210     184.348 175.383  18.375  1.00 13.93      A
C
ATOM    734  CG  LEU A 210     185.046 176.317  17.381  1.00 16.57      A
C
ATOM    735  CD1 LEU A 210     186.507 175.915  17.264  1.00 14.44      A
C
ATOM    736  CD2 LEU A 210     184.351 176.245  16.022  1.00 12.75      A
C
ATOM    737  C   LEU A 210     182.464 174.731  19.841  1.00 10.33      A
C
ATOM    738  O   LEU A 210     182.591 174.664  21.053  1.00 14.25      A
O
ATOM    739  N   GLU A 211     181.784 173.843  19.139  1.00 11.52      A
N
ATOM    740  CA  GLU A 211     181.218 172.646  19.739  1.00 12.06      A
C
ATOM    741  CB  GLU A 211     180.272 171.970  18.751  1.00 15.25      A
C
ATOM    742  CG  GLU A 211     180.147 170.462  18.927  1.00 16.63      A
C
ATOM    743  CD  GLU A 211     179.379 169.783  17.784  1.00 23.31      A
C
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ATOM    744  OE1 GLU A 211     179.201 168.531  17.837  1.00 22.59           A
O
ATOM    745  OE2 GLU A 211     178.954 170.500  16.829  1.00 22.15           A
O
ATOM    746  C   GLU A 211     182.424 171.723  20.009  1.00 14.58           A
C
ATOM    747  O   GLU A 211     183.296 171.561  19.156  1.00 11.41           A
O
ATOM    748  N   TYR A 212     182.466 171.133  21.196  1.00 13.40           A
N
ATOM    749  CA  TYR A 212     183.555 170.247  21.589  1.00 15.01           A
C
ATOM    750  CB  TYR A 212     183.541 170.072  23.108  1.00 16.32           A
C
ATOM    751  CG  TYR A 212     184.387 168.938  23.679  1.00 18.16           A
C
ATOM    752  CD1 TYR A 212     185.744 168.820  23.391  1.00 15.83           A
C
ATOM    753  CE1 TYR A 212     186.528 167.845  24.013  1.00 16.35           A
C
ATOM    754  CD2 TYR A 212     183.829 168.042  24.601  1.00 18.49           A
C
ATOM    755  CE2 TYR A 212     184.590 167.074  25.223  1.00 16.40           A
C
ATOM    756  CZ  TYR A 212     185.934 166.973  24.934  1.00 19.22           A
C
ATOM    757  OH  TYR A 212     186.655 165.995  25.594  1.00 15.81           A
O
ATOM    758  C   TYR A 212     183.463 168.889  20.909  1.00 15.14           A
C
ATOM    759  O   TYR A 212     182.414 168.259  20.920  1.00 14.66           A
O
ATOM    760  N   ALA A 213     184.561 168.451  20.297  1.00 15.74           A
N
ATOM    761  CA  ALA A 213     184.623 167.142  19.636  1.00 14.66           A
C
ATOM    762  CB  ALA A 213     185.341 167.270  18.302  1.00 16.59           A
C
ATOM    763  C   ALA A 213     185.417 166.270  20.615  1.00 16.61           A
C
ATOM    764  O   ALA A 213     186.638 166.352  20.682  1.00 16.21           A
O
ATOM    765  N   PRO A 214     184.724 165.418  21.380  1.00 15.97           A
N
ATOM    766  CD  PRO A 214     183.323 165.077  21.082  1.00 15.58           A
C
ATOM    767  CA  PRO A 214     185.258 164.515  22.398  1.00 15.31           A
C
ATOM    768  CB  PRO A 214     184.000 163.837  22.963  1.00 14.60           A
C
ATOM    769  CG  PRO A 214     182.844 164.624  22.417  1.00 17.26           A
C
ATOM    770  C   PRO A 214     186.319 163.472  22.000  1.00 17.90           A
C
ATOM    771  O   PRO A 214     187.172 163.152  22.829  1.00 18.00           A
O
ATOM    772  N   LEU A 215     186.274 162.922  20.777  1.00 14.95           A
N
ATOM    773  CA  LEU A 215     187.214 161.880  20.362  1.00 14.66           A
C
ATOM    774  CB  LEU A 215     186.453 160.710  19.692  1.00 16.00           A
C
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ATOM    775  CG  LEU A 215     185.316 160.072  20.536  1.00 22.00      A
C
ATOM    776  CD1 LEU A 215     184.664 158.818  19.898  1.00 17.85      A
C
ATOM    777  CD2 LEU A 215     185.906 159.717  21.877  1.00 20.55      A
C
ATOM    778  C   LEU A 215     188.415 162.306  19.505  1.00 14.59      A
C
ATOM    779  O   LEU A 215     189.093 161.477  18.905  1.00 14.29      A
O
ATOM    780  N   GLY A 216     188.691 163.603  19.455  1.00 16.74      A
N
ATOM    781  CA  GLY A 216     189.836 164.070  18.694  1.00 14.83      A
C
ATOM    782  C   GLY A 216     189.701 164.060  17.184  1.00 13.54      A
C
ATOM    783  O   GLY A 216     188.597 164.008  16.656  1.00 12.48      A
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ATOM    784  N   THR A 217     190.843 164.091  16.497  1.00 12.97      A
N
ATOM    785  CA  THR A 217     190.867 164.136  15.044  1.00 14.08      A
C
ATOM    786  CB  THR A 217     192.005 164.998  14.503  1.00 14.49      A
C
ATOM    787  OG1 THR A 217     193.242 164.310  14.733  1.00 16.68      A
O
ATOM    788  CG2 THR A 217     192.043 166.347  15.167  1.00 10.84      A
C
ATOM    789  C   THR A 217     191.060 162.811  14.347  1.00 16.46      A
C
ATOM    790  O   THR A 217     191.741 161.910  14.849  1.00 15.02      A
O
ATOM    791  N   VAL A 218     190.481 162.721  13.153  1.00 16.27      A
N
ATOM    792  CA  VAL A 218     190.616 161.533  12.340  1.00 15.99      A
C
ATOM    793  CB  VAL A 218     189.802 161.683  11.038  1.00 16.57      A
C
ATOM    794  CG1 VAL A 218     190.263 160.649   9.999  1.00 18.56      A
C
ATOM    795  CG2 VAL A 218     188.339 161.504  11.349  1.00 11.27      A
C
ATOM    796  C   VAL A 218     192.117 161.366  12.051  1.00 16.41      A
C
ATOM    797  O   VAL A 218     192.611 160.255  11.896  1.00 15.84      A
O
ATOM    798  N   TYR A 219     192.826 162.487  12.008  1.00 15.85      A
N
ATOM    799  CA  TYR A 219     194.261 162.509  11.789  1.00 16.76      A
C
ATOM    800  CB  TYR A 219     194.771 163.937  11.908  1.00 18.52      A
C
ATOM    801  CG  TYR A 219     196.259 164.024  11.800  1.00 19.33      A
C
ATOM    802  CD1 TYR A 219     196.870 163.870  10.570  1.00 17.55      A
C
ATOM    803  CE1 TYR A 219     198.249 163.929  10.450  1.00 23.59      A
C
ATOM    804  CD2 TYR A 219     197.065 164.236  12.936  1.00 21.27      A
C
ATOM    805  CE2 TYR A 219     198.454 164.289  12.834  1.00 20.92      A
C
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ATOM    806  CZ  TYR A 219     199.032 164.136  11.584  1.00 24.53      A
C
ATOM    807  OH  TYR A 219     200.392 164.188  11.448  1.00 28.22      A
O
ATOM    808  C   TYR A 219     194.999 161.661  12.826  1.00 18.49      A
C
ATOM    809  O   TYR A 219     195.910 160.888  12.494  1.00 18.32      A
O
ATOM    810  N   ARG A 220     194.617 161.836  14.086  1.00 16.66      A
N
ATOM    811  CA  ARG A 220     195.247 161.100  15.154  1.00 19.76      A
C
ATOM    812  CB  ARG A 220     194.848 161.674  16.514  1.00 22.26      A
C
ATOM    813  CG  ARG A 220     195.514 160.949  17.669  1.00 27.26      A
C
ATOM    814  CD  ARG A 220     197.039 161.124  17.660  1.00 29.11      A
C
ATOM    815  NE  ARG A 220     197.689 160.200  18.595  1.00 32.84      A
N
ATOM    816  CZ  ARG A 220     199.003 160.005  18.702  1.00 35.53      A
C
ATOM    817  NH1 ARG A 220     199.867 160.669  17.931  1.00 39.53      A
N
ATOM    818  NH2 ARG A 220     199.449 159.129  19.594  1.00 36.11      A
N
ATOM    819  C   ARG A 220     194.908 159.608  15.088  1.00 19.85      A
C
ATOM    820  O   ARG A 220     195.768 158.748  15.322  1.00 19.84      A
O
ATOM    821  N   GLU A 221     193.661 159.309  14.746  1.00 19.44      A
N
ATOM    822  CA  GLU A 221     193.192 157.935  14.628  1.00 21.14      A
C
ATOM    823  CB  GLU A 221     191.670 157.930  14.386  1.00 22.94      A
C
ATOM    824  CG  GLU A 221     190.968 156.594  14.519  1.00 27.24      A
C
ATOM    825  CD  GLU A 221     191.078 155.998  15.918  1.00 30.92      A
C
ATOM    826  OE1 GLU A 221     190.736 154.798  16.073  1.00 35.57      A
O
ATOM    827  OE2 GLU A 221     191.502 156.716  16.857  1.00 31.40      A
O
ATOM    828  C   GLU A 221     193.930 157.268  13.465  1.00 22.03      A
C
ATOM    829  O   GLU A 221     194.201 156.061  13.493  1.00 21.79      A
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ATOM    830  N   LEU A 222     194.257 158.060  12.442  1.00 20.91      A
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ATOM    831  CA  LEU A 222     194.969 157.533  11.287  1.00 18.01      A
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ATOM    832  CB  LEU A 222     194.838 158.485  10.079  1.00 17.83      A
C
ATOM    833  CG  LEU A 222     195.181 157.923   8.676  1.00 21.87      A
C
ATOM    834  CD1 LEU A 222     194.366 156.652   8.358  1.00 17.44      A
C
ATOM    835  CD2 LEU A 222     194.892 159.007   7.634  1.00 19.79      A
C
ATOM    836  C   LEU A 222     196.439 157.261  11.639  1.00 16.91      A
C
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ATOM    837  O   LEU A 222     197.012 156.317  11.119  1.00 16.89      A
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ATOM    838  N   GLN A 223     197.062 158.066  12.503  1.00 16.66      A
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ATOM    839  CA  GLN A 223     198.446 157.769  12.900  1.00 17.24      A
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ATOM    840  CB  GLN A 223     199.022 158.808  13.850  1.00 19.18      A
C
ATOM    841  CG  GLN A 223     199.250 160.205  13.317  1.00 28.34      A
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ATOM    842  CD  GLN A 223     199.954 161.058  14.355  1.00 31.88      A
C
ATOM    843  OE1 GLN A 223     199.437 161.241  15.474  1.00 31.86      A
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ATOM    844  NE2 GLN A 223     201.149 161.584  14.005  1.00 34.43      A
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ATOM    845  C   GLN A 223     198.456 156.448  13.688  1.00 21.01      A
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ATOM    846  O   GLN A 223     199.360 155.630  13.523  1.00 18.77      A
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ATOM    847  N   LYS A 224     197.464 156.277  14.570  1.00 21.30      A
N
ATOM    848  CA  LYS A 224     197.357 155.099  15.419  1.00 21.07      A
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ATOM    849  CB  LYS A 224     196.258 155.300  16.492  1.00 24.80      A
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ATOM    850  CG  LYS A 224     196.479 156.522  17.399  1.00 26.43      A
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ATOM    851  CD  LYS A 224     195.427 156.642  18.505  1.00 30.49      A
C
ATOM    852  CE  LYS A 224     195.834 157.727  19.507  1.00 31.44      A
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ATOM    853  NZ  LYS A 224     194.917 157.868  20.668  1.00 33.32      A
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ATOM    854  C   LYS A 224     197.088 153.812  14.647  1.00 20.29      A
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ATOM    855  O   LYS A 224     197.799 152.829  14.821  1.00 19.90      A
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ATOM    856  N   LEU A 225     196.059 153.800  13.806  1.00 20.45      A
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ATOM    857  CA  LEU A 225     195.753 152.603  13.039  1.00 18.46      A
C
ATOM    858  CB  LEU A 225     194.272 152.588  12.615  1.00 20.03      A
C
ATOM    859  CG  LEU A 225     193.224 152.691  13.740  1.00 24.89      A
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ATOM    860  CD1 LEU A 225     191.784 152.656  13.213  1.00 20.57      A
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ATOM    861  CD2 LEU A 225     193.462 151.543  14.674  1.00 26.58      A
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ATOM    862  C   LEU A 225     196.631 152.464  11.780  1.00 19.83      A
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ATOM    863  O   LEU A 225     196.694 151.381  11.186  1.00 20.09      A
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ATOM    864  N   SER A 226     197.296 153.545  11.375  1.00 18.33      A
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ATOM    865  CA  SER A 226     198.137 153.578  10.158  1.00 21.51      A
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ATOM    866  CB  SER A 226     199.160 152.426  10.124  1.00 21.48      A
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ATOM    867  OG  SER A 226     200.116 152.533  11.177  1.00 27.63      A
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ATOM	869	O	SER	A	226	197.566	154.284	7.927	1.00	19.41	A
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ATOM	870	N	LYS	A	227	196.290	152.664	8.838	1.00	20.02	A
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ATOM	871	CA	LYS	A	227	195.358	152.524	7.697	1.00	19.86	A
C											
ATOM	872	CB	LYS	A	227	195.668	151.280	6.876	1.00	24.72	A
C											
ATOM	873	CG	LYS	A	227	196.854	151.364	5.990	1.00	29.64	A
C											
ATOM	874	CD	LYS	A	227	197.148	149.990	5.419	1.00	35.21	A
C											
ATOM	875	CE	LYS	A	227	198.330	150.088	4.465	1.00	41.32	A
C											
ATOM	876	NZ	LYS	A	227	198.843	148.758	4.016	1.00	43.82	A
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ATOM	877	C	LYS	A	227	193.970	152.303	8.274	1.00	16.62	A
C											
ATOM	878	O	LYS	A	227	193.852	151.881	9.411	1.00	18.80	A
O											
ATOM	879	N	PHE	A	228	192.930	152.584	7.499	1.00	14.54	A
N											
ATOM	880	CA	PHE	A	228	191.548	152.342	7.932	1.00	15.70	A
C											
ATOM	881	CB	PHE	A	228	190.665	153.590	7.729	1.00	12.09	A
C											
ATOM	882	CG	PHE	A	228	190.958	154.697	8.679	1.00	13.97	A
C											
ATOM	883	CD1	PHE	A	228	190.564	156.005	8.400	1.00	14.03	A
C											
ATOM	884	CD2	PHE	A	228	191.629	154.439	9.860	1.00	13.49	A
C											
ATOM	885	CE1	PHE	A	228	190.844	157.046	9.299	1.00	12.37	A
C											
ATOM	886	CE2	PHE	A	228	191.912	155.466	10.767	1.00	14.79	A
C											
ATOM	887	CZ	PHE	A	228	191.520	156.772	10.487	1.00	11.50	A
C											
ATOM	888	C	PHE	A	228	191.051	151.227	7.016	1.00	15.70	A
C											
ATOM	889	O	PHE	A	228	191.399	151.212	5.833	1.00	16.89	A
O											
ATOM	890	N	ASP	A	229	190.261	150.290	7.536	1.00	16.61	A
N											
ATOM	891	CA	ASP	A	229	189.753	149.221	6.666	1.00	18.23	A
C											
ATOM	892	CB	ASP	A	229	189.261	148.005	7.478	1.00	17.42	A
C											
ATOM	893	CG	ASP	A	229	188.092	148.325	8.369	1.00	20.41	A
C											
ATOM	894	OD1	ASP	A	229	187.161	149.024	7.930	1.00	28.20	A
O											
ATOM	895	OD2	ASP	A	229	188.072	147.859	9.511	1.00	26.24	A
O											
ATOM	896	C	ASP	A	229	188.624	149.817	5.810	1.00	16.57	A
C											
ATOM	897	O	ASP	A	229	188.322	151.006	5.939	1.00	17.37	A
O											
ATOM	898	N	GLU	A	230	187.998	149.020	4.952	1.00	15.33	A
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ATOM    902  CD  GLU A 230     187.313 147.497   0.794  1.00 27.22      A
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ATOM    903  OE1 GLU A 230     186.584 146.478   0.753  1.00 28.49      A
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ATOM    904  OE2 GLU A 230     187.711 148.085  -0.244  1.00 29.45      A
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ATOM    905  C   GLU A 230     185.680 150.062   4.783  1.00 16.70      A
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ATOM    906  O   GLU A 230     185.141 151.099   4.419  1.00 13.33      A
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ATOM    907  N   GLN A 231     185.209 149.326   5.782  1.00 16.53      A
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ATOM    908  CA  GLN A 231     184.003 149.711   6.512  1.00 17.02      A
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ATOM    909  CB  GLN A 231     183.728 148.656   7.596  1.00 15.32      A
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ATOM    910  CG  GLN A 231     182.370 148.737   8.289  1.00 17.56      A
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ATOM    911  CD  GLN A 231     182.297 149.841   9.359  1.00 22.59      A
C
ATOM    912  OE1 GLN A 231     183.298 150.112  10.075  1.00 21.11      A
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ATOM    913  NE2 GLN A 231     181.106 150.478   9.494  1.00 19.70      A
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ATOM    914  C   GLN A 231     184.195 151.124   7.120  1.00 17.00      A
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ATOM    915  O   GLN A 231     183.381 152.024   6.890  1.00 18.40      A
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ATOM    916  N   ARG A 232     185.281 151.308   7.873  1.00 17.36      A
N
ATOM    917  CA  ARG A 232     185.607 152.593   8.509  1.00 17.63      A
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ATOM    918  CB  ARG A 232     186.905 152.465   9.307  1.00 19.87      A
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ATOM    919  CG  ARG A 232     187.205 153.647  10.172  1.00 20.99      A
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ATOM    920  CD  ARG A 232     186.795 153.359  11.597  1.00 28.38      A
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ATOM    921  NE  ARG A 232     187.588 154.189  12.487  1.00 32.23      A
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ATOM    922  CZ  ARG A 232     188.247 153.745  13.545  1.00 31.41      A
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ATOM    923  NH1 ARG A 232     188.213 152.459  13.873  1.00 29.13      A
N
ATOM    924  NH2 ARG A 232     188.963 154.604  14.257  1.00 35.98      A
N
ATOM    925  C   ARG A 232     185.770 153.747   7.507  1.00 14.94      A
C
ATOM    926  O   ARG A 232     185.356 154.866   7.761  1.00 12.98      A
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ATOM    928  CA  THR A 233     186.652 154.446   5.361  1.00 13.60      A
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ATOM    929  CB  THR A 233     187.719 153.902   4.340  1.00 14.55      A
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ATOM	930	OG1	THR	A	233	188.937	153.623	5.048	1.00	14.87	A
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C											
ATOM	932	C	THR	A	233	185.339	154.863	4.686	1.00	13.47	A
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ATOM	933	O	THR	A	233	185.090	156.056	4.508	1.00	12.81	A
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ATOM	934	N	ALA	A	234	184.481	153.901	4.353	1.00	11.54	A
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C											
ATOM	936	CB	ALA	A	234	182.531	152.967	3.184	1.00	6.31	A
C											
ATOM	937	C	ALA	A	234	182.254	154.953	4.675	1.00	15.13	A
C											
ATOM	938	O	ALA	A	234	181.498	155.843	4.272	1.00	18.25	A
O											
ATOM	939	N	THR	A	235	182.297	154.579	5.945	1.00	13.08	A
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ATOM	940	CA	THR	A	235	181.450	155.221	6.909	1.00	11.34	A
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ATOM	941	CB	THR	A	235	181.581	154.543	8.289	1.00	13.04	A
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ATOM	942	OG1	THR	A	235	181.181	153.167	8.177	1.00	13.03	A
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ATOM	943	CG2	THR	A	235	180.679	155.235	9.304	1.00	9.30	A
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ATOM	944	C	THR	A	235	181.813	156.701	6.976	1.00	12.76	A
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ATOM	945	O	THR	A	235	180.930	157.553	6.894	1.00	14.21	A
O											
ATOM	946	N	TYR	A	236	183.104	157.003	7.115	1.00	12.83	A
N											
ATOM	947	CA	TYR	A	236	183.586	158.392	7.157	1.00	14.72	A
C											
ATOM	948	CB	TYR	A	236	185.096	158.451	7.371	1.00	16.17	A
C											
ATOM	949	CG	TYR	A	236	185.572	158.175	8.772	1.00	16.12	A
C											
ATOM	950	CD1	TYR	A	236	184.785	158.491	9.876	1.00	16.03	A
C											
ATOM	951	CE1	TYR	A	236	185.237	158.261	11.162	1.00	16.90	A
C											
ATOM	952	CD2	TYR	A	236	186.830	157.626	8.993	1.00	13.79	A
C											
ATOM	953	CE2	TYR	A	236	187.290	157.397	10.266	1.00	15.98	A
C											
ATOM	954	CZ	TYR	A	236	186.490	157.709	11.347	1.00	19.04	A
C											
ATOM	955	OH	TYR	A	236	186.935	157.420	12.609	1.00	22.33	A
O											
ATOM	956	C	TYR	A	236	183.291	159.154	5.862	1.00	16.50	A
C											
ATOM	957	O	TYR	A	236	182.873	160.311	5.898	1.00	15.39	A
O											
ATOM	958	N	ILE	A	237	183.536	158.517	4.718	1.00	14.99	A
N											
ATOM	959	CA	ILE	A	237	183.274	159.176	3.456	1.00	15.34	A
C											
ATOM	960	CB	ILE	A	237	183.656	158.295	2.242	1.00	15.72	A
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ATOM 963 CD1 ILE A 237 186.062 159.254 2.278 1.00 13.67 A
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ATOM 964 C ILE A 237 181.795 159.542 3.379 1.00 17.56 A
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ATOM 965 O ILE A 237 181.442 160.638 2.953 1.00 18.55 A
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ATOM 969 OG1 THR A 238 179.059 156.502 3.464 1.00 16.26 A
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ATOM 970 CG2 THR A 238 177.257 157.817 4.354 1.00 13.58 A
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ATOM 972 O THR A 238 178.214 160.829 4.307 1.00 14.27 A
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ATOM 975 CB GLU A 239 179.913 161.025 8.170 1.00 14.00 A
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ATOM 976 CG GLU A 239 179.443 159.721 8.804 1.00 18.38 A
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ATOM 977 CD GLU A 239 180.121 159.365 10.124 1.00 24.00 A
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ATOM 978 OE1 GLU A 239 181.366 159.259 10.187 1.00 24.67 A
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ATOM 979 OE2 GLU A 239 179.385 159.158 11.114 1.00 32.52 A
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ATOM 980 C GLU A 239 179.767 162.548 6.149 1.00 13.27 A
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ATOM 981 O GLU A 239 179.028 163.525 6.073 1.00 12.45 A
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ATOM 982 N LEU A 240 181.005 162.538 5.668 1.00 11.05 A
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ATOM 983 CA LEU A 240 181.566 163.707 5.049 1.00 13.29 A
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ATOM 984 CB LEU A 240 183.043 163.465 4.738 1.00 15.79 A
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ATOM 985 CG LEU A 240 183.894 164.638 4.235 1.00 16.19 A
C
ATOM 986 CD1 LEU A 240 184.031 165.720 5.279 1.00 19.17 A
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ATOM 987 CD2 LEU A 240 185.267 164.108 3.884 1.00 19.04 A
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ATOM 988 C LEU A 240 180.798 164.081 3.773 1.00 13.39 A
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ATOM 989 O LEU A 240 180.513 165.256 3.548 1.00 14.19 A
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ATOM 990 N ALA A 241 180.443 163.091 2.955 1.00 11.67 A
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ATOM 991 CA ALA A 241 179.726 163.372 1.711 1.00 12.50 A
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ATOM    997  CB  ASN A 242     175.822 163.329   4.619  1.00 20.05      A
C
ATOM    998  CG  ASN A 242     175.213 162.005   4.210  1.00 22.16      A
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ATOM   1011  CG  LEU A 244     181.958 167.607   1.791  1.00 13.66      A
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ATOM   1012  CD1 LEU A 244     182.862 166.784   0.883  1.00 10.60      A
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ATOM   1013  CD2 LEU A 244     182.570 168.990   2.068  1.00 10.59      A
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ATOM   1014  C   LEU A 244     178.245 168.764   1.078  1.00 13.84      A
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ATOM   1016  N   SER A 245     177.363 167.776   0.949  1.00 11.65      A
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ATOM   1017  CA  SER A 245     176.162 167.951   0.149  1.00 12.45      A
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ATOM   1018  CB  SER A 245     175.403 166.623   0.101  1.00 11.63      A
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ATOM   1019  OG  SER A 245     174.265 166.724  -0.729  1.00 18.58      A
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ATOM   1021  O   SER A 245     174.753 169.925  -0.028  1.00 13.38      A
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ATOM   1024  CB  TYR A 246     174.337 169.838   4.232  1.00 10.92      A
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ATOM   1026  CD1 TYR A 246     172.615 171.398   5.169  1.00 11.79      A
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ATOM   1027  CE1 TYR A 246     172.249 172.526   5.886  1.00 15.75      A
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ATOM   1028  CD2 TYR A 246     174.905 171.782   5.727  1.00 14.34      A
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ATOM   1029  CE2 TYR A 246     174.548 172.925   6.452  1.00 17.65      A
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ATOM   1036  CB  CYS A 247     178.697 172.339   2.453  1.00 18.30      A
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ATOM   1037  SG  CYS A 247     179.389 172.397   4.097  1.00 20.02      A
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ATOM   1038  C   CYS A 247     177.033 173.298   0.930  1.00 14.64      A
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ATOM   1042  CB  HIS A 248     177.246 171.711  -2.361  1.00 14.58      A
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ATOM   1043  CG  HIS A 248     178.698 171.388  -2.305  1.00 15.75      A
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ATOM   1044  CD2 HIS A 248     179.651 171.777  -1.427  1.00 14.69      A
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ATOM   1045  ND1 HIS A 248     179.331 170.596  -3.236  1.00 18.18      A
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ATOM   1046  CE1 HIS A 248     180.614 170.512  -2.934  1.00 15.22      A
C
ATOM   1047  NE2 HIS A 248     180.832 171.220  -1.840  1.00 14.77      A
N
ATOM   1048  C   HIS A 248     175.474 173.338  -1.717  1.00 16.00      A
C
ATOM   1049  O   HIS A 248     175.285 174.228  -2.538  1.00 16.44      A
O
ATOM   1050  N   SER A 249     174.503 172.744  -1.028  1.00 14.49      A
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ATOM   1051  CA  SER A 249     173.125 173.148  -1.197  1.00 15.32      A
C
ATOM   1052  CB  SER A 249     172.201 172.233  -0.392  1.00 11.40      A
C
ATOM   1053  OG  SER A 249     172.281 172.527   0.985  1.00 16.48      A
O
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ATOM   1054  C   SER A 249     173.055 174.597  -0.696  1.00 16.09      A
C
ATOM   1055  O   SER A 249     172.139 175.350  -1.034  1.00 18.04      A
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ATOM   1056  N   LYS A 250     174.031 174.988   0.118  1.00 15.99      A
N
ATOM   1057  CA  LYS A 250     174.072 176.363   0.599  1.00 15.13      A
C
ATOM   1058  CB  LYS A 250     174.405 176.441   2.107  1.00 13.57      A
C
ATOM   1059  CG  LYS A 250     173.350 175.850   3.040  1.00 15.19      A
C
ATOM   1060  CD  LYS A 250     171.930 176.203   2.629  1.00 19.05      A
C
ATOM   1061  CE  LYS A 250     170.943 175.150   3.131  1.00 24.43      A
C
ATOM   1062  NZ  LYS A 250     169.492 175.372   2.776  1.00 28.76      A
N
ATOM   1063  C   LYS A 250     175.106 177.133  -0.210  1.00 11.97      A
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ATOM   1064  O   LYS A 250     175.375 178.286    .957  1.00 14.99      A
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ATOM   1065  N   ARG A 251     175.686 176.478  -1.208  1.00 14.14      A
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ATOM   1066  CA  ARG A 251     176.690 177.099  -2.079  1.00 13.45      A
C
ATOM   1067  CB  ARG A 251     176.080 178.305  -2.792  1.00 14.05      A
C
ATOM   1068  CG  ARG A 251     174.976 177.936  -3.779  1.00 21.06      A
C
ATOM   1069  CD  ARG A 251     175.441 178.112  -5.227  1.00 27.95      A
C
ATOM   1070  NE  ARG A 251     175.547 176.844  -5.943  1.00 31.22      A
N
ATOM   1071  CZ  ARG A 251     176.391 176.615  -6.949  1.00 31.35      A
C
ATOM   1072  NH1 ARG A 251     177.214 177.570  -7.368  1.00 28.63      A
N
ATOM   1073  NH2 ARG A 251     176.427 175.422  -7.526  1.00 31.96      A
N
ATOM   1074  C   ARG A 251     177.974 177.493  -1.362  1.00 12.30      A
C
ATOM   1075  O   ARG A 251     178.618 178.472  -1.703  1.00 12.69      A
O
ATOM   1076  N   VAL A 252     178.344 176.714  -0.363  1.00 11.12      A
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ATOM   1077  CA  VAL A 252     179.569 176.971   0.368  1.00 12.45      A
C
ATOM   1078  CB  VAL A 252     179.338 176.810   1.885  1.00 12.23      A
C
ATOM   1079  CG1 VAL A 252     180.651 176.509   2.587  1.00  9.08      A
C
ATOM   1080  CG2 VAL A 252     178.681 178.059   2.446  1.00 10.54      A
C
ATOM   1081  C   VAL A 252     180.604 175.940  -0.083  1.00 15.27      A
C
ATOM   1082  O   VAL A 252     180.267 174.774  -0.265  1.00 12.78      A
O
ATOM   1083  N   ILE A 253     181.840 176.373  -0.326  1.00 13.72      A
N
ATOM   1084  CA  ILE A 253     182.872 175.419  -0.680  1.00 10.89      A
C
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ATOM 1085 CB ILE A 253 183.670 175.788 -1.957 1.00 11.67 A
C
ATOM 1086 CG2 ILE A 253 184.426 174.535 -2.441 1.00 5.83 A
C
ATOM 1087 CG1 ILE A 253 182.733 176.323 -3.059 1.00 10.28 A
C
ATOM 1088 CD1 ILE A 253 183.439 176.812 -4.329 1.00 3.57 A
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ATOM 1089 C ILE A 253 183.831 175.453 0.498 1.00 13.01 A
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ATOM 1090 O ILE A 253 184.347 176.524 0.849 1.00 13.11 A
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ATOM 1091 N HIS A 254 184.050 174.288 1.113 1.00 13.19 A
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ATOM 1092 CA HIS A 254 184.943 174.161 2.259 1.00 12.95 A
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ATOM 1093 CB HIS A 254 184.868 172.745 2.843 1.00 12.70 A
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ATOM 1094 CG HIS A 254 185.587 172.606 4.160 1.00 12.92 A
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ATOM 1095 CD2 HIS A 254 185.206 172.914 5.423 1.00 9.91 A
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ATOM 1096 ND1 HIS A 254 186.898 172.180 4.257 1.00 13.73 A
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ATOM 1097 CE1 HIS A 254 187.290 172.229 5.515 1.00 10.14 A
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ATOM 1098 NE2 HIS A 254 186.282 172.671 6.243 1.00 11.29 A
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ATOM 1099 C HIS A 254 186.383 174.507 1.889 1.00 13.04 A
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ATOM 1100 O HIS A 254 186.971 175.438 2.447 1.00 14.41 A
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ATOM 1101 N ARG A 255 186.935 173.743 0.953 1.00 12.07 A
N
ATOM 1102 CA ARG A 255 188.291 173.910 0.438 1.00 12.35 A
C
ATOM 1103 CB ARG A 255 188.494 175.341 -0.050 1.00 13.05 A
C
ATOM 1104 CG ARG A 255 187.553 175.664 -1.200 1.00 15.96 A
C
ATOM 1105 CD ARG A 255 187.942 176.885 -1.997 1.00 11.42 A
C
ATOM 1106 NE ARG A 255 188.045 178.075 -1.183 1.00 13.42 A
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ATOM 1107 CZ ARG A 255 188.194 179.295 -1.690 1.00 17.97 A
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ATOM 1108 NH1 ARG A 255 188.248 179.453 -3.012 1.00 12.59 A
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ATOM 1109 NH2 ARG A 255 188.308 180.348 -0.880 1.00 11.08 A
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ATOM 1110 C ARG A 255 189.479 173.491 1.328 1.00 14.82 A
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ATOM 1111 O ARG A 255 190.628 173.656 0.914 1.00 16.45 A
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ATOM 1113 CA ASP A 256 190.355 172.522 3.364 1.00 14.13 A
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ATOM 1114 CB ASP A 256 190.779 173.631 4.341 1.00 15.61 A
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ATOM 1115 CG ASP A 256 192.185 173.408 4.930 1.00 17.71 A
C

ATOM 1116 OD1 ASP A 256 193.119 172.950 4.217 1.00 18.23 A
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ATOM 1117 OD2 ASP A 256 192.364 173.712 6.130 1.00 20.01 A
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ATOM 1118 C ASP A 256 190.021 171.231 4.094 1.00 14.83 A
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ATOM 1119 O ASP A 256 190.209 171.088 5.300 1.00 17.90 A
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ATOM 1120 N ILE A 257 189.522 170.285 3.321 1.00 14.83 A
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ATOM 1121 CA ILE A 257 189.170 168.978 3.809 1.00 15.89 A
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ATOM 1122 CB ILE A 257 188.209 168.318 2.821 1.00 16.68 A
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ATOM 1123 CG2 ILE A 257 188.096 166.834 3.106 1.00 18.21 A
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ATOM 1124 CG1 ILE A 257 186.851 169.010 2.909 1.00 19.11 A
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ATOM 1125 CD1 ILE A 257 185.939 168.636 1.771 1.00 26.98 A
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ATOM 1126 C ILE A 257 190.461 168.170 3.888 1.00 16.84 A
C
ATOM 1127 O ILE A 257 191.180 168.019 2.890 1.00 19.23 A
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ATOM 1128 N LYS A 258 190.759 167.673 5.079 1.00 14.42 A
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ATOM 1129 CA LYS A 258 191.948 166.861 5.321 1.00 13.61 A
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ATOM 1130 CB LYS A 258 193.218 167.696 5.165 1.00 11.12 A
C
ATOM 1131 CG LYS A 258 193.288 168.912 6.021 1.00 10.35 A
C
ATOM 1132 CD LYS A 258 194.685 169.397 5.941 1.00 11.98 A
C
ATOM 1133 CE LYS A 258 194.946 170.539 6.844 1.00 10.31 A
C
ATOM 1134 NZ LYS A 258 196.316 171.028 6.523 1.00 13.12 A
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ATOM 1135 C LYS A 258 191.828 166.275 6.728 1.00 12.82 A
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ATOM 1136 O LYS A 258 191.093 166.807 7.565 1.00 12.94 A
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ATOM 1137 N PRO A 259 192.547 165.180 7.011 1.00 13.48 A
N
ATOM 1138 CD PRO A 259 193.607 164.582 6.181 1.00 11.93 A
C
ATOM 1139 CA PRO A 259 192.487 164.525 8.329 1.00 14.07 A
C
ATOM 1140 CB PRO A 259 193.641 163.517 8.267 1.00 14.89 A
C
ATOM 1141 CG PRO A 259 193.714 163.197 6.778 1.00 14.98 A
C
ATOM 1142 C PRO A 259 192.527 165.413 9.583 1.00 15.36 A
C
ATOM 1143 O PRO A 259 191.773 165.171 10.520 1.00 15.88 A
O
ATOM 1144 N GLU A 260 193.388 166.428 9.593 1.00 15.22 A
N
ATOM 1145 CA GLU A 260 193.516 167.340 10.734 1.00 19.96 A
C
ATOM 1146 CB GLU A 260 194.770 168.225 10.563 1.00 22.41 A
C

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ATOM   1147  CG  GLU A 260     196.090 167.457  10.516  1.00 29.11      A
C
ATOM   1148  CD  GLU A 260     196.610 167.140   9.092  1.00 32.88      A
C
ATOM   1149  OE1 GLU A 260     195.826 166.656   8.235  1.00 33.12      A
O
ATOM   1150  OE2 GLU A 260     197.823 167.360   8.841  1.00 35.49      A
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ATOM   1151  C   GLU A 260     192.280 168.252  10.924  1.00 18.80      A
C
ATOM   1152  O   GLU A 260     192.140 168.905  11.957  1.00 18.71      A
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ATOM   1153  N   ASN A 261     191.401 168.309   9.922  1.00 16.14      A
N
ATOM   1154  CA  ASN A 261     190.206 169.139  10.014  1.00 14.12      A
C
ATOM   1155  CB  ASN A 261     190.084 170.036   8.799  1.00 12.74      A
C
ATOM   1156  CG  ASN A 261     191.068 171.176   8.824  1.00 12.37      A
C
ATOM   1157  OD1 ASN A 261     191.719 171.446   9.840  1.00 11.65      A
O
ATOM   1158  ND2 ASN A 261     191.178 171.868   7.705  1.00 11.18      A
N
ATOM   1159  C   ASN A 261     188.944 168.329  10.159  1.00 14.87      A
C
ATOM   1160  O   ASN A 261     187.844 168.855  10.027  1.00 14.12      A
O
ATOM   1161  N   LEU A 262     189.117 167.037  10.428  1.00 16.20      A
N
ATOM   1162  CA  LEU A 262     187.996 166.127  10.596  1.00 13.58      A
C
ATOM   1163  CB  LEU A 262     188.128 164.954   9.627  1.00 13.22      A
C
ATOM   1164  CG  LEU A 262     188.164 165.406   8.162  1.00 15.01      A
C
ATOM   1165  CD1 LEU A 262     188.502 164.230   7.232  1.00  8.10      A
C
ATOM   1166  CD2 LEU A 262     186.807 166.049   7.834  1.00 10.56      A
C
ATOM   1167  C   LEU A 262     188.027 165.633  12.031  1.00 15.43      A
C
ATOM   1168  O   LEU A 262     188.999 165.008  12.459  1.00 17.59      A
O
ATOM   1169  N   LEU A 263     186.968 165.915  12.777  1.00 11.89      A
N
ATOM   1170  CA  LEU A 263     186.926 165.505  14.154  1.00 10.46      A
C
ATOM   1171  CB  LEU A 263     186.657 166.725  15.005  1.00 13.46      A
C
ATOM   1172  CG  LEU A 263     187.584 167.921  14.699  1.00 14.28      A
C
ATOM   1173  CD1 LEU A 263     187.208 169.055  15.634  1.00 15.02      A
C
ATOM   1174  CD2 LEU A 263     189.050 167.563  14.865  1.00 12.28      A
C
ATOM   1175  C   LEU A 263     185.905 164.407  14.409  1.00 12.75      A
C
ATOM   1176  O   LEU A 263     185.068 164.112  13.553  1.00 13.83      A
O
ATOM   1177  N   LEU A 264     185.989 163.780  15.576  1.00 13.44      A
N
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ATOM   1178  CA  LEU A 264     185.076 162.693  15.919  1.00 15.08      A
C
ATOM   1179  CB  LEU A 264     185.856 161.421  16.298  1.00 15.27      A
C
ATOM   1180  CG  LEU A 264     186.808 160.821  15.263  1.00 16.94      A
C
ATOM   1181  CD1 LEU A 264     187.393 159.499  15.783  1.00 20.04      A
C
ATOM   1182  CD2 LEU A 264     186.043 160.590  13.944  1.00 16.69      A
C
ATOM   1183  C   LEU A 264     184.190 163.103  17.078  1.00 14.83      A
C
ATOM   1184  O   LEU A 264     184.669 163.613  18.096  1.00 13.07      A
O
ATOM   1185  N   GLY A 265     182.890 162.881  16.907  1.00 14.85      A
N
ATOM   1186  CA  GLY A 265     181.943 163.218  17.947  1.00 15.69      A
C
ATOM   1187  C   GLY A 265     181.844 162.127  18.999  1.00 17.48      A
C
ATOM   1188  O   GLY A 265     182.597 161.144  18.989  1.00 19.40      A
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ATOM   1189  N   SER A 266     180.888 162.306  19.899  1.00 17.64      A
N
ATOM   1190  CA  SER A 266     180.641 161.398  21.007  1.00 18.83      A
C
ATOM   1191  CB  SER A 266     179.417 161.895  21.766  1.00 17.49      A
C
ATOM   1192  OG  SER A 266     179.347 161.294  23.037  1.00 31.06      A
O
ATOM   1193  C   SER A 266     180.457 159.923  20.615  1.00 16.59      A
C
ATOM   1194  O   SER A 266     180.771 159.025  21.389  1.00 16.64      A
O
ATOM   1195  N   ALA A 267     179.960 159.675  19.412  1.00 15.97      A
N
ATOM   1196  CA  ALA A 267     179.731 158.314  18.939  1.00 17.67      A
C
ATOM   1197  CB  ALA A 267     178.288 158.163  18.456  1.00 14.65      A
C
ATOM   1198  C   ALA A 267     180.670 157.930  17.815  1.00 18.92      A
C
ATOM   1199  O   ALA A 267     180.353 157.040  17.025  1.00 21.00      A
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N
ATOM   1201  CA  GLY A 268     182.741 158.278  16.648  1.00 22.38      A
C
ATOM   1202  C   GLY A 268     182.289 158.773  15.282  1.00 21.15      A
C
ATOM   1203  O   GLY A 268     182.809 158.323  14.266  1.00 20.78      A
O
ATOM   1204  N   GLU A 269     181.324 159.690  15.249  1.00 19.71      A
N
ATOM   1205  CA  GLU A 269     180.831 160.239  13.983  1.00 18.83      A
C
ATOM   1206  CB  GLU A 269     179.386 160.746  14.107  1.00 20.11      A
C
ATOM   1207  CG  GLU A 269     179.239 162.020  14.944  1.00 27.28      A
C
ATOM   1208  CD  GLU A 269     178.874 161.722  16.385  1.00 29.04      A
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ATOM   1209  OE1 GLU A 269     179.762 161.324  17.177  1.00 30.97      A
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ATOM   1210  OE2 GLU A 269     177.677 161.868  16.711  1.00 33.63      A
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ATOM   1211  C   GLU A 269     181.702 161.409  13.549  1.00 17.27      A
C
ATOM   1212  O   GLU A 269     182.088 162.249  14.368  1.00 15.38      A
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ATOM   1213  N   LEU A 270     181.994 161.461  12.253  1.00 14.97      A
N
ATOM   1214  CA  LEU A 270     182.822 162.515  11.689  1.00 15.39      A
C
ATOM   1215  CB  LEU A 270     183.169 162.167  10.229  1.00 21.78      A
C
ATOM   1216  CG  LEU A 270     184.100 163.071   9.408  1.00 22.18      A
C
ATOM   1217  CD1 LEU A 270     185.484 162.839   9.938  1.00 26.73      A
C
ATOM   1218  CD2 LEU A 270     184.109 162.725   7.944  1.00 27.39      A
C
ATOM   1219  C   LEU A 270     182.129 163.876  11.722  1.00 13.13      A
C
ATOM   1220  O   LEU A 270     180.932 163.973  11.490  1.00 12.45      A
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ATOM   1221  N   LYS A 271     182.895 164.918  12.027  1.00 13.69      A
N
ATOM   1222  CA  LYS A 271     182.395 166.296  12.025  1.00 13.80      A
C
ATOM   1223  CB  LYS A 271     182.201 166.814  13.450  1.00 13.22      A
C
ATOM   1224  CG  LYS A 271     180.846 166.378  14.025  1.00 16.86      A
C
ATOM   1225  CD  LYS A 271     180.790 166.428  15.509  1.00 17.04      A
C
ATOM   1226  CE  LYS A 271     179.494 165.823  15.967  1.00 15.79      A
C
ATOM   1227  NZ  LYS A 271     178.379 166.692  15.545  1.00 20.81      A
N
ATOM   1228  C   LYS A 271     183.392 167.151  11.270  1.00 15.22      A
C
ATOM   1229  O   LYS A 271     184.586 167.152  11.582  1.00 16.95      A
O
ATOM   1230  N   ILE A 272     182.919 167.842  10.238  1.00 15.55      A
N
ATOM   1231  CA  ILE A 272     183.803 168.702   9.462  1.00 15.61      A
C
ATOM   1232  CB  ILE A 272     183.143 169.220   8.163  1.00 19.61      A
C
ATOM   1233  CG2 ILE A 272     184.054 170.269   7.530  1.00 18.20      A
C
ATOM   1234  CG1 ILE A 272     182.850 168.069   7.203  1.00 22.81      A
C
ATOM   1235  CD1 ILE A 272     182.068 168.504   5.967  1.00 25.62      A
C
ATOM   1236  C   ILE A 272     184.051 169.926  10.303  1.00 13.27      A
C
ATOM   1237  O   ILE A 272     183.136 170.422  10.945  1.00 12.04      A
O
ATOM   1238  N   ALA A 273     185.270 170.428  10.294  1.00 11.17      A
N
ATOM   1239  CA  ALA A 273     185.568 171.623  11.069  1.00 13.73      A
C
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ATOM   1240  CB  ALA A 273     186.266 171.248  12.376  1.00 10.14      A
C
ATOM   1241  C   ALA A 273     186.472 172.498  10.225  1.00 16.38      A
C
ATOM   1242  O   ALA A 273     186.688 172.208   9.047  1.00 16.96      A
O
ATOM   1243  N   ASP A 274     186.986 173.568  10.834  1.00 17.04      A
N
ATOM   1244  CA  ASP A 274     187.913 174.500  10.200  1.00 15.18      A
C
ATOM   1245  CB  ASP A 274     189.288 173.805  10.074  1.00 17.02      A
C
ATOM   1246  CG  ASP A 274     190.447 174.786   9.800  1.00 19.27      A
C
ATOM   1247  OD1 ASP A 274     190.190 175.999   9.635  1.00 22.45      A
O
ATOM   1248  OD2 ASP A 274     191.624 174.338   9.753  1.00 17.87      A
O
ATOM   1249  C   ASP A 274     187.434 175.064   8.838  1.00 16.14      A
C
ATOM   1250  O   ASP A 274     187.846 174.604   7.776  1.00 12.68      A
O
ATOM   1251  N   PHE A 275     186.559 176.065   8.881  1.00 15.86      A
N
ATOM   1252  CA  PHE A 275     186.074 176.688   7.666  1.00 14.12      A
C
ATOM   1253  CB  PHE A 275     184.602 177.108   7.835  1.00 13.16      A
C
ATOM   1254  CG  PHE A 275     183.640 175.948   7.721  1.00 12.72      A
C
ATOM   1255  CD1 PHE A 275     183.540 174.994   8.746  1.00 11.42      A
C
ATOM   1256  CD2 PHE A 275     182.936 175.727   6.535  1.00 11.44      A
C
ATOM   1257  CE1 PHE A 275     182.768 173.843   8.581  1.00 10.04      A
C
ATOM   1258  CE2 PHE A 275     182.157 174.568   6.367  1.00 12.57      A
C
ATOM   1259  CZ  PHE A 275     182.079 173.631   7.396  1.00 11.15      A
C
ATOM   1260  C   PHE A 275     186.966 177.868   7.289  1.00 15.87      A
C
ATOM   1261  O   PHE A 275     186.541 178.780   6.568  1.00 15.07      A
O
ATOM   1262  N   GLY A 276     188.221 177.820   7.751  1.00 15.09      A
N
ATOM   1263  CA  GLY A 276     189.184 178.875   7.452  1.00 17.20      A
C
ATOM   1264  C   GLY A 276     189.322 179.285   5.983  1.00 16.44      A
C
ATOM   1265  O   GLY A 276     189.368 180.482   5.665  1.00 17.13      A
O
ATOM   1266  N   TRP A 277     189.378 178.307   5.082  1.00 13.73      A
N
ATOM   1267  CA  TRP A 277     189.514 178.596   3.664  1.00 14.40      A
C
ATOM   1268  CB  TRP A 277     190.568 177.667   3.071  1.00 20.13      A
C
ATOM   1269  CG  TRP A 277     191.860 177.753   3.789  1.00 22.40      A
C
ATOM   1270  CD2 TRP A 277     192.691 178.904   3.893  1.00 23.73      A
C
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ATOM   1271  CE2 TRP A 277     193.788 178.558   4.701  1.00 26.05      A
C
ATOM   1272  CE3 TRP A 277     192.617 180.198   3.375  1.00 25.94      A
C
ATOM   1273  CD1 TRP A 277     192.463 176.777   4.517  1.00 23.25      A
C
ATOM   1274  NE1 TRP A 277     193.625 177.250   5.074  1.00 24.53      A
N
ATOM   1275  CZ2 TRP A 277     194.806 179.467   5.015  1.00 27.86      A
C
ATOM   1276  CZ3 TRP A 277     193.631 181.106   3.686  1.00 28.74      A
C
ATOM   1277  CH2 TRP A 277     194.711 180.733   4.496  1.00 26.68      A
C
ATOM   1278  C   TRP A 277     188.202 178.467   2.888  1.00 13.46      A
C
ATOM   1279  O   TRP A 277     188.190 178.362   1.664  1.00 14.44      A
O
ATOM   1280  N   SER A 278     187.097 178.481   3.605  1.00 14.67      A
N
ATOM   1281  CA  SER A 278     185.809 178.360   2.973  1.00 16.81      A
C
ATOM   1282  CB  SER A 278     184.785 177.937   4.009  1.00 18.65      A
C
ATOM   1283  OG  SER A 278     185.042 176.588   4.334  1.00 31.56      A
O
ATOM   1284  C   SER A 278     185.338 179.620   2.269  1.00 15.59      A
C
ATOM   1285  O   SER A 278     185.887 180.700   2.456  1.00 13.40      A
O
ATOM   1286  N   VAL A 279     184.330 179.468   1.427  1.00 12.47      A
N
ATOM   1287  CA  VAL A 279     183.790 180.622   0.750  1.00 15.04      A
C
ATOM   1288  CB  VAL A 279     184.631 181.010  -0.524  1.00 14.76      A
C
ATOM   1289  CG1 VAL A 279     184.436 179.985  -1.646  1.00 10.49      A
C
ATOM   1290  CG2 VAL A 279     184.256 182.419  -0.971  1.00  9.51      A
C
ATOM   1291  C   VAL A 279     182.347 180.399   0.352  1.00 15.66      A
C
ATOM   1292  O   VAL A 279     181.902 179.259   0.162  1.00 16.74      A
O
ATOM   1293  N   HIS A 280     181.604 181.491   0.276  1.00 14.84      A
N
ATOM   1294  CA  HIS A 280     180.224 181.389  -0.133  1.00 17.48      A
C
ATOM   1295  CB  HIS A 280     179.332 182.330   0.694  1.00 14.36      A
C
ATOM   1296  CG  HIS A 280     177.885 182.230   0.336  1.00 16.95      A
C
ATOM   1297  CD2 HIS A 280     177.154 181.176  -0.102  1.00 16.10      A
C
ATOM   1298  ND1 HIS A 280     177.045 183.323   0.300  1.00 15.76      A
N
ATOM   1299  CE1 HIS A 280     175.864 182.946  -0.154  1.00 17.22      A
C
ATOM   1300  NE2 HIS A 280     175.903 181.648  -0.407  1.00 18.56      A
N
ATOM   1301  C   HIS A 280     180.236 181.772  -1.622  1.00 17.74      A
C
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ATOM   1302  O   HIS A 280     180.439 182.942  -1.989  1.00 16.22      A
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ATOM   1303  N   ALA A 281     180.048 180.773  -2.480  1.00 15.79      A
N
ATOM   1304  CA  ALA A 281     180.066 180.984  -3.930  1.00 17.35      A
C
ATOM   1305  CB  ALA A 281     181.103 180.047  -4.565  1.00 15.43      A
C
ATOM   1306  C   ALA A 281     178.693 180.779  -4.610  1.00 18.31      A
C
ATOM   1307  O   ALA A 281     178.489 179.809  -5.311  1.00 18.09      A
O
ATOM   1308  N   PRO A 282     177.754 181.726  -4.412  1.00 20.27      A
N
ATOM   1309  CD  PRO A 282     177.983 182.946  -3.597  1.00 20.44      A
C
ATOM   1310  CA  PRO A 282     176.381 181.701  -4.974  1.00 21.92      A
C
ATOM   1311  CB  PRO A 282     175.770 183.032  -4.483  1.00 21.47      A
C
ATOM   1312  CG  PRO A 282     176.575 183.413  -3.327  1.00 21.85      A
C
ATOM   1313  C   PRO A 282     176.326 181.581  -6.480  1.00 22.24      A
C
ATOM   1314  O   PRO A 282     175.611 180.729  -6.987  1.00 24.89      A
O
ATOM   1315  N   SER A 283     177.088 182.439  -7.163  1.00 24.90      A
N
ATOM   1316  CA  SER A 283     177.131 182.464  -8.629  1.00 28.30      A
C
ATOM   1317  CB  SER A 283     176.711 183.837  -9.202  1.00 26.31      A
C
ATOM   1318  OG  SER A 283     175.659 184.461  -8.492  1.00 30.72      A
O
ATOM   1319  C   SER A 283     178.454 182.133  -9.327  1.00 27.14      A
C
ATOM   1320  O   SER A 283     178.563 181.133 -10.033  1.00 31.35      A
O
ATOM   1321  N   SER A 284     179.434 183.011  -9.147  1.00 25.92      A
N
ATOM   1322  CA  SER A 284     180.749 182.937  -9.789  1.00 26.41      A
C
ATOM   1323  CB  SER A 284     181.476 184.252  -9.583  1.00 26.11      A
C
ATOM   1324  OG  SER A 284     180.590 185.288  -9.231  1.00 32.06      A
O
ATOM   1325  C   SER A 284     181.720 181.869  -9.346  1.00 24.70      A
C
ATOM   1326  O   SER A 284     181.617 181.347  -8.254  1.00 26.06      A
O
ATOM   1327  N   ARG A 285     182.717 181.636 -10.192  1.00 23.60      A
N
ATOM   1328  CA  ARG A 285     183.782 180.701  -9.910  1.00 25.00      A
C
ATOM   1329  CB  ARG A 285     184.337 180.169 -11.225  1.00 25.95      A
C
ATOM   1330  CG  ARG A 285     183.367 179.201 -11.935  1.00 31.00      A
C
ATOM   1331  CD  ARG A 285     184.154 178.152 -12.746  1.00 38.12      A
C
ATOM   1332  NE  ARG A 285     184.419 178.543 -14.135  1.00 42.96      A
N
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ATOM   1333  CZ  ARG A 285     185.202 177.856 -14.971  1.00 45.91      A
C
ATOM   1334  NH1 ARG A 285     185.808 176.744 -14.560  1.00 46.53      A
N
ATOM   1335  NH2 ARG A 285     185.364 178.267 -16.225  1.00 46.52      A
N
ATOM   1336  C   ARG A 285     184.869 181.436  -9.074  1.00 23.19      A
C
ATOM   1337  O   ARG A 285     184.791 182.652  -8.873  1.00 23.63      A
O
ATOM   1338  N   ARG A 286     185.871 180.720  -8.578  1.00 22.25      A
N
ATOM   1339  CA  ARG A 286     186.898 181.369  -7.770  1.00 18.11      A
C
ATOM   1340  CB  ARG A 286     186.781 180.826  -6.344  1.00 16.41      A
C
ATOM   1341  CG  ARG A 286     185.467 181.252  -5.671  1.00 17.03      A
C
ATOM   1342  CD  ARG A 286     185.642 182.655  -5.179  1.00 16.99      A
C
ATOM   1343  NE  ARG A 286     184.443 183.221  -4.632  1.00 25.38      A
N
ATOM   1344  CZ  ARG A 286     184.398 184.417  -4.072  1.00 26.94      A
C
ATOM   1345  NH1 ARG A 286     185.509 185.138  -3.995  1.00 28.48      A
N
ATOM   1346  NH2 ARG A 286     183.244 184.894  -3.605  1.00 30.62      A
N
ATOM   1347  C   ARG A 286     188.309 181.189  -8.339  1.00 19.47      A
C
ATOM   1348  O   ARG A 286     188.537 180.305  -9.174  1.00 17.62      A
O
ATOM   1349  N   TPO A 287     189.226 182.041  -7.916  1.00 21.77      A
N
ATOM   1350  CA  TPO A 287     190.558 181.974  -8.377  1.00 21.28      A
C
ATOM   1351  CB  TPO A 287     190.775 183.306  -9.113  1.00 25.22      A
C
ATOM   1352  CG2 TPO A 287     189.942 183.372 -10.421  1.00 22.17      A
C
ATOM   1353  OG1 TPO A 287     190.484 184.557  -8.448  1.00 33.29      A
O
ATOM   1354  P   TPO A 287     191.582 185.763  -8.444  1.00 33.70      A
P
ATOM   1355  O1P TPO A 287     190.902 186.991  -9.195  1.00 41.17      A
O
ATOM   1356  O2P TPO A 287     192.847 185.199  -9.239  1.00 37.62      A
O
ATOM   1357  O3P TPO A 287     191.990 186.067  -6.912  1.00 41.70      A
O
ATOM   1358  C   TPO A 287     191.612 181.717  -7.265  1.00 16.99      A
C
ATOM   1359  O   TPO A 287     192.886 181.536  -7.600  1.00 25.86      A
O
ATOM   1360  N   TPO A 288     191.139 181.614  -6.033  1.00 16.91      A
N
ATOM   1361  CA  TPO A 288     192.066 181.441  -4.938  1.00 16.31      A
C
ATOM   1362  CB  TPO A 288     191.262 181.750  -3.672  1.00 18.77      A
C
ATOM   1363  CG2 TPO A 288     192.190 181.949  -2.512  1.00 16.50      A
C
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ATOM   1364  OG1 TPO A 288     190.694 183.015  -3.936  1.00 23.64      A
O
ATOM   1365  P   TPO A 288     189.163 183.188  -3.329  1.00 18.56      A
P
ATOM   1366  O1P TPO A 288     189.234 182.723  -1.818  1.00 19.25      A
O
ATOM   1367  O2P TPO A 288     188.217 182.242  -4.154  1.00 24.67      A
O
ATOM   1368  O3P TPO A 288     188.820 184.760  -3.320  1.00 24.29      A
O
ATOM   1369  C   TPO A 288     192.828 180.109  -4.873  1.00 17.62      A
C
ATOM   1370  O   TPO A 288     192.132 178.986  -5.036  1.00 16.48      A
O
ATOM   1371  N   LEU A 289     194.152 180.122  -4.825  1.00 19.62      A
N
ATOM   1372  CA  LEU A 289     194.793 178.875  -4.419  1.00 20.29      A
C
ATOM   1373  CB  LEU A 289     196.229 178.759  -4.993  1.00 21.71      A
C
ATOM   1374  CG  LEU A 289     196.977 177.458  -4.598  1.00 25.59      A
C
ATOM   1375  CD1 LEU A 289     196.506 176.298  -5.488  1.00 30.17      A
C
ATOM   1376  CD2 LEU A 289     198.475 177.596  -4.769  1.00 26.69      A
C
ATOM   1377  C   LEU A 289     194.833 178.800  -2.900  1.00 17.60      A
C
ATOM   1378  O   LEU A 289     195.428 179.646  -2.272  1.00 20.61      A
O
ATOM   1379  N   CYS A 290     194.191 177.810  -2.307  1.00 16.97      A
N
ATOM   1380  CA  CYS A 290     194.204 177.679  -0.844  1.00 18.91      A
C
ATOM   1381  CB  CYS A 290     193.102 178.535  -0.201  1.00 16.86      A
C
ATOM   1382  SG  CYS A 290     191.434 178.234  -0.820  1.00 22.10      A
S
ATOM   1383  C   CYS A 290     194.003 176.211  -0.453  1.00 17.81      A
C
ATOM   1384  O   CYS A 290     193.554 175.403  -1.266  1.00 15.28      A
O
ATOM   1385  N   GLY A 291     194.340 175.862   0.786  1.00 19.11      A
N
ATOM   1386  CA  GLY A 291     194.203 174.484   1.227  1.00 18.98      A
C
ATOM   1387  C   GLY A 291     195.536 173.896   1.644  1.00 19.71      A
C
ATOM   1388  O   GLY A 291     196.458 174.606   2.047  1.00 21.01      A
O
ATOM   1389  N   THR A 292     195.626 172.584   1.523  1.00 18.60      A
N
ATOM   1390  CA  THR A 292     196.800 171.837   1.903  1.00 16.87      A
C
ATOM   1391  CB  THR A 292     196.378 170.657   2.760  1.00 19.75      A
C
ATOM   1392  OG1 THR A 292     195.457 171.126   3.752  1.00 25.57      A
O
ATOM   1393  CG2 THR A 292     197.563 169.991   3.407  1.00 18.64      A
C
ATOM   1394  C   THR A 292     197.453 171.308   0.652  1.00 17.38      A
C
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ATOM   1395  O   THR A 292     196.772 170.864  -0.269  1.00 16.20      A
O
ATOM   1396  N   LEU A 293     198.780 171.347   0.631  1.00 18.38      A
N
ATOM   1397  CA  LEU A 293     199.545 170.868  -0.511  1.00 18.67      A
C
ATOM   1398  CB  LEU A 293     201.011 170.747  -0.102  1.00 18.33      A
C
ATOM   1399  CG  LEU A 293     201.947 170.217  -1.188  1.00 19.70      A
C
ATOM   1400  CD1 LEU A 293     201.997 171.229  -2.316  1.00 20.14      A
C
ATOM   1401  CD2 LEU A 293     203.332 169.962  -0.603  1.00 18.52      A
C
ATOM   1402  C   LEU A 293     199.063 169.533  -1.126  1.00 19.06      A
C
ATOM   1403  O   LEU A 293     198.654 169.496  -2.287  1.00 16.78      A
O
ATOM   1404  N   ASP A 294     199.106 168.447  -0.355  1.00 16.52      A
N
ATOM   1405  CA  ASP A 294     198.701 167.143  -0.868  1.00 15.08      A
C
ATOM   1406  CB  ASP A 294     199.029 166.048   0.164  1.00 19.73      A
C
ATOM   1407  CG  ASP A 294     200.527 165.669   0.175  1.00 23.92      A
C
ATOM   1408  OD1 ASP A 294     201.065 165.254  -0.891  1.00 23.94      A
O
ATOM   1409  OD2 ASP A 294     201.161 165.783   1.245  1.00 24.71      A
O
ATOM   1410  C   ASP A 294     197.239 167.026  -1.309  1.00 14.50      A
C
ATOM   1411  O   ASP A 294     196.875 166.084  -2.011  1.00 11.76      A
O
ATOM   1412  N   TYR A 295     196.411 167.996  -0.923  1.00 13.78      A
N
ATOM   1413  CA  TYR A 295     194.993 167.963  -1.267  1.00 12.35      A
C
ATOM   1414  CB  TYR A 295     194.156 168.157  -0.001  1.00 12.74      A
C
ATOM   1415  CG  TYR A 295     194.061 166.933   0.868  1.00 16.79      A
C
ATOM   1416  CD1 TYR A 295     195.179 166.449   1.561  1.00 19.00      A
C
ATOM   1417  CE1 TYR A 295     195.119 165.265   2.307  1.00 18.70      A
C
ATOM   1418  CD2 TYR A 295     192.871 166.216   0.947  1.00 16.93      A
C
ATOM   1419  CE2 TYR A 295     192.792 165.035   1.682  1.00 21.69      A
C
ATOM   1420  CZ  TYR A 295     193.916 164.559   2.357  1.00 22.19      A
C
ATOM   1421  OH  TYR A 295     193.805 163.362   3.046  1.00 26.24      A
O
ATOM   1422  C   TYR A 295     194.542 168.963  -2.336  1.00 10.66      A
C
ATOM   1423  O   TYR A 295     193.387 168.955  -2.741  1.00 11.85      A
O
ATOM   1424  N   LEU A 296     195.460 169.797  -2.805  1.00 10.92      A
N
ATOM   1425  CA  LEU A 296     195.119 170.800  -3.807  1.00 13.78      A
C
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ATOM   1426  CB  LEU A 296     196.328 171.679  -4.144  1.00 11.44      A
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ATOM   1427  CG  LEU A 296     196.931 172.488  -2.995  1.00 15.78      A
C
ATOM   1428  CD1 LEU A 296     198.287 173.081  -3.411  1.00 13.74      A
C
ATOM   1429  CD2 LEU A 296     195.954 173.585  -2.582  1.00 15.05      A
C
ATOM   1430  C   LEU A 296     194.591 170.206  -5.108  1.00 14.17      A
C
ATOM   1431  O   LEU A 296     195.144 169.255  -5.648  1.00 12.20      A
O
ATOM   1432  N   PRO A 297     193.504 170.783  -5.631  1.00 13.56      A
N
ATOM   1433  CD  PRO A 297     192.676 171.841  -5.015  1.00 13.83      A
C
ATOM   1434  CA  PRO A 297     192.921 170.302  -6.893  1.00 12.38      A
C
ATOM   1435  CB  PRO A 297     191.516 170.923  -6.872  1.00 14.10      A
C
ATOM   1436  CG  PRO A 297     191.744 172.233  -6.155  1.00 13.16      A
C
ATOM   1437  C   PRO A 297     193.772 170.826  -8.083  1.00 14.86      A
C
ATOM   1438  O   PRO A 297     194.361 171.906  -7.993  1.00 14.20      A
O
ATOM   1439  N   PRO A 298     193.830 170.080  -9.213  1.00 14.90      A
N
ATOM   1440  CD  PRO A 298     193.074 168.838  -9.478  1.00 13.08      A
C
ATOM   1441  CA  PRO A 298     194.606 170.479 -10.403  1.00 12.06      A
C
ATOM   1442  CB  PRO A 298     194.228 169.428 -11.450  1.00 12.23      A
C
ATOM   1443  CG  PRO A 298     193.813 168.254 -10.653  1.00 11.96      A
C
ATOM   1444  C   PRO A 298     194.250 171.874 -10.894  1.00 12.75      A
C
ATOM   1445  O   PRO A 298     195.124 172.677 -11.218  1.00 12.47      A
O
ATOM   1446  N   GLU A 299     192.954 172.154 -10.954  1.00 12.43      A
N
ATOM   1447  CA  GLU A 299     192.495 173.447 -11.427  1.00 15.93      A
C
ATOM   1448  CB  GLU A 299     190.956 173.520 -11.439  1.00 15.99      A
C
ATOM   1449  CG  GLU A 299     190.283 173.211 -10.098  1.00 20.28      A
C
ATOM   1450  CD  GLU A 299     189.893 171.729  -9.951  1.00 22.71      A
C
ATOM   1451  OE1 GLU A 299     190.741 170.854 -10.262  1.00 22.72      A
O
ATOM   1452  OE2 GLU A 299     188.743 171.450  -9.525  1.00 19.63      A
O
ATOM   1453  C   GLU A 299     193.068 174.609 -10.615  1.00 17.99      A
C
ATOM   1454  O   GLU A 299     193.217 175.706 -11.147  1.00 21.24      A
O
ATOM   1455  N   MET A 300     193.385 174.401  -9.340  1.00 17.80      A
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ATOM   1456  CA  MET A 300     193.949 175.497  -8.541  1.00 21.17      A
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ATOM   1457  CB  MET A 300     193.781 175.248  -7.031  1.00 21.87      A
C
ATOM   1458  CG  MET A 300     192.562 175.935  -6.417  1.00 24.58      A
C
ATOM   1459  SD  MET A 300     192.223 175.516  -4.665  1.00 23.96      A
S
ATOM   1460  CE  MET A 300     193.835 175.427  -4.097  1.00 25.92      A
C
ATOM   1461  C   MET A 300     195.429 175.697  -8.845  1.00 22.52      A
C
ATOM   1462  O   MET A 300     195.900 176.818  -9.034  1.00 17.97      A
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ATOM   1463  N   ILE A 301     196.153 174.592  -8.905  1.00 25.70      A
N
ATOM   1464  CA  ILE A 301     197.573 174.627  -9.160  1.00 28.05      A
C
ATOM   1465  CB  ILE A 301     198.162 173.192  -9.173  1.00 31.23      A
C
ATOM   1466  CG2 ILE A 301     199.640 173.228  -9.502  1.00 33.00      A
C
ATOM   1467  CG1 ILE A 301     197.977 172.525  -7.813  1.00 34.03      A
C
ATOM   1468  CD1 ILE A 301     198.227 171.019  -7.871  1.00 39.59      A
C
ATOM   1469  C   ILE A 301     197.857 175.289 -10.501  1.00 28.39      A
C
ATOM   1470  O   ILE A 301     198.736 176.140 -10.608  1.00 28.70      A
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ATOM   1471  N   GLU A 302     197.091 174.902 -11.513  1.00 29.15      A
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ATOM   1472  CA  GLU A 302     197.260 175.411 -12.864  1.00 27.63      A
C
ATOM   1473  CB  GLU A 302     196.614 174.449 -13.847  1.00 28.51      A
C
ATOM   1474  CG  GLU A 302     197.309 173.128 -13.932  1.00 31.90      A
C
ATOM   1475  CD  GLU A 302     196.442 172.074 -14.604  1.00 34.88      A
C
ATOM   1476  OE1 GLU A 302     195.546 172.441 -15.420  1.00 35.44      A
O
ATOM   1477  OE2 GLU A 302     196.663 170.878 -14.322  1.00 33.88      A
O
ATOM   1478  C   GLU A 302     196.759 176.817 -13.160  1.00 26.56      A
C
ATOM   1479  O   GLU A 302     196.730 177.216 -14.323  1.00 25.45      A
O
ATOM   1480  N   GLY A 303     196.351 177.553 -12.130  1.00 26.68      A
N
ATOM   1481  CA  GLY A 303     195.891 178.915 -12.333  1.00 24.63      A
C
ATOM   1482  C   GLY A 303     194.576 179.072 -13.077  1.00 26.17      A
C
ATOM   1483  O   GLY A 303     194.333 180.080 -13.739  1.00 25.60      A
O
ATOM   1484  N   ARG A 304     193.718 178.068 -12.976  1.00 27.24      A
N
ATOM   1485  CA  ARG A 304     192.409 178.095 -13.617  1.00 26.83      A
C
ATOM   1486  CB  ARG A 304     192.068 176.721 -14.229  1.00 26.35      A
C
ATOM   1487  CG  ARG A 304     192.726 176.410 -15.584  1.00 35.40      A
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ATOM   1488  CD  ARG A 304     191.737 176.691 -16.749  1.00 43.36      A
C
ATOM   1489  NE  ARG A 304     192.316 176.665 -18.095  1.00 47.14      A
N
ATOM   1490  CZ  ARG A 304     191.602 176.827 -19.210  1.00 51.59      A
C
ATOM   1491  NH1 ARG A 304     190.290 177.025 -19.121  1.00 54.10      A
N
ATOM   1492  NH2 ARG A 304     192.189 176.794 -20.413  1.00 53.71      A
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ATOM   1494  O   ARG A 304     191.684 178.391 -11.326  1.00 29.71      A
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ATOM   1496  CA  MET A 305     189.112 179.048 -12.038  1.00 26.17      A
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ATOM   1497  CB  MET A 305     188.027 179.807 -12.757  1.00 30.29      A
C
ATOM   1498  CG  MET A 305     188.517 181.155 -13.154  1.00 35.60      A
C
ATOM   1499  SD  MET A 305     187.192 182.156 -13.740  1.00 46.48      A
S
ATOM   1500  CE  MET A 305     187.949 182.896 -15.291  1.00 45.95      A
C
ATOM   1501  C   MET A 305     188.544 177.772 -11.466  1.00 23.39      A
C
ATOM   1502  O   MET A 305     188.653 176.721 -12.082  1.00 23.54      A
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ATOM   1503  N   HIS A 306     187.934 177.852 -10.290  1.00 21.16      A
N
ATOM   1504  CA  HIS A 306     187.363 176.655  -9.703  1.00 17.32      A
C
ATOM   1505  CB  HIS A 306     188.312 176.035  -8.671  1.00 15.79      A
C
ATOM   1506  CG  HIS A 306     188.498 176.853  -7.431  1.00 14.36      A
C
ATOM   1507  CD2 HIS A 306     187.895 176.788  -6.218  1.00 12.29      A
C
ATOM   1508  ND1 HIS A 306     189.411 177.880  -7.347  1.00 15.91      A
N
ATOM   1509  CE1 HIS A 306     189.366 178.411  -6.139  1.00 13.45      A
C
ATOM   1510  NE2 HIS A 306     188.453 177.767  -5.434  1.00 10.38      A
N
ATOM   1511  C   HIS A 306     186.000 176.913  -9.078  1.00 18.65      A
C
ATOM   1512  O   HIS A 306     185.528 178.063  -9.040  1.00 15.46      A
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N
ATOM   1514  CA  ASP A 307     184.057 175.824  -7.986  1.00 20.30      A
C
ATOM   1515  CB  ASP A 307     182.969 175.631  -9.035  1.00 24.34      A
C
ATOM   1516  CG  ASP A 307     183.174 174.374  -9.865  1.00 30.83      A
C
ATOM   1517  OD1 ASP A 307     183.553 173.321  -9.286  1.00 33.25      A
O
ATOM   1518  OD2 ASP A 307     182.949 174.430 -11.098  1.00 33.88      A
O
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ATOM   1519  C   ASP A 307     183.948 174.721  -6.917  1.00 19.00      A
C
ATOM   1520  O   ASP A 307     184.973 174.176  -6.486  1.00 21.60      A
O
ATOM   1521  N   GLU A 308     182.720 174.368  -6.519  1.00 18.46      A
N
ATOM   1522  CA  GLU A 308     182.507 173.358  -5.479  1.00 17.19      A
C
ATOM   1523  CB  GLU A 308     181.014 173.257  -5.075  1.00 19.78      A
C
ATOM   1524  CG  GLU A 308     180.067 172.849  -6.190  1.00 29.00      A
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ATOM   1527  OE2 GLU A 308     177.910 171.836  -6.115  1.00 41.55      A
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ATOM   1528  C   GLU A 308     183.048 171.977  -5.820  1.00 14.99      A
C
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O
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N
ATOM   1531  CA  LYS A 309     183.997 170.488  -7.449  1.00 16.26      A
C
ATOM   1532  CB  LYS A 309     184.061 170.376  -8.972  1.00 18.82      A
C
ATOM   1533  CG  LYS A 309     182.731 170.086  -9.593  1.00 21.29      A
C
ATOM   1534  CD  LYS A 309     182.215 168.769  -9.041  1.00 29.52      A
C
ATOM   1535  CE  LYS A 309     181.020 168.263  -9.842  1.00 30.17      A
C
ATOM   1536  NZ  LYS A 309     180.649 166.912  -9.358  1.00 35.57      A
N
ATOM   1537  C   LYS A 309     185.370 170.202  -6.826  1.00 16.49      A
C
ATOM   1538  O   LYS A 309     185.816 169.051  -6.804  1.00 15.73      A
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ATOM   1539  N   VAL A 310     186.025 171.233  -6.291  1.00 15.44      A
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ATOM   1540  CA  VAL A 310     187.319 171.020  -5.662  1.00 13.90      A
C
ATOM   1541  CB  VAL A 310     188.051 172.358  -5.281  1.00 15.52      A
C
ATOM   1542  CG1 VAL A 310     188.197 173.247  -6.503  1.00  7.36      A
C
ATOM   1543  CG2 VAL A 310     187.332 173.065  -4.151  1.00 12.70      A
C
ATOM   1544  C   VAL A 310     187.132 170.159  -4.410  1.00 17.23      A
C
ATOM   1545  O   VAL A 310     188.008 169.357  -4.083  1.00 19.39      A
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ATOM   1546  N   ASP A 311     186.013 170.306  -3.700  1.00 14.90      A
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ATOM   1547  CA  ASP A 311     185.804 169.452  -2.541  1.00 14.20      A
C
ATOM   1548  CB  ASP A 311     184.574 169.876  -1.727  1.00 16.81      A
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ATOM   1549  CG  ASP A 311     184.778 171.192  -0.974  1.00 16.28      A
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ATOM   1550  OD1 ASP A 311     185.950 171.565  -0.731  1.00 12.12      A
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ATOM   1551  OD2 ASP A 311     183.756 171.832  -0.617  1.00 13.33      A
O
ATOM   1552  C   ASP A 311     185.640 167.983  -2.979  1.00 14.98      A
C
ATOM   1553  O   ASP A 311     185.953 167.090  -2.202  1.00 16.71      A
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ATOM   1556  CB  LEU A 312     184.238 166.279  -6.028  1.00 12.75      A
C
ATOM   1557  CG  LEU A 312     182.708 166.216  -6.008  1.00 16.02      A
C
ATOM   1558  CD1 LEU A 312     182.269 164.959  -5.273  1.00 14.12      A
C
ATOM   1559  CD2 LEU A 312     182.118 167.482  -5.336  1.00 16.09      A
C
ATOM   1560  C   LEU A 312     186.399 165.749  -4.951  1.00 13.94      A
C
ATOM   1561  O   LEU A 312     186.616 164.546  -4.837  1.00 15.77      A
O
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N
ATOM   1563  CA  TRP A 313     188.673 166.093  -5.553  1.00 13.67      A
C
ATOM   1564  CB  TRP A 313     189.505 167.131  -6.287  1.00 10.13      A
C
ATOM   1565  CG  TRP A 313     190.948 166.889  -6.208  1.00  9.91      A
C
ATOM   1566  CD2 TRP A 313     191.775 166.296  -7.214  1.00 11.32      A
C
ATOM   1567  CE2 TRP A 313     193.109 166.370  -6.750  1.00 10.99      A
C
ATOM   1568  CE3 TRP A 313     191.523 165.729  -8.471  1.00  8.98      A
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ATOM   1569  CD1 TRP A 313     191.784 167.266  -5.199  1.00 10.59      A
C
ATOM   1570  NE1 TRP A 313     193.083 166.960  -5.513  1.00  9.03      A
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ATOM   1571  CZ2 TRP A 313     194.190 165.890  -7.494  1.00 10.17      A
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ATOM   1572  CZ3 TRP A 313     192.598 165.254  -9.214  1.00 13.43      A
C
ATOM   1573  CH2 TRP A 313     193.923 165.344  -8.723  1.00 12.05      A
C
ATOM   1574  C   TRP A 313     189.258 165.776  -4.183  1.00 12.20      A
C
ATOM   1575  O   TRP A 313     189.803 164.704  -3.983  1.00 11.38      A
O
ATOM   1576  N   SER A 314     189.111 166.700  -3.236  1.00 13.68      A
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ATOM   1577  CA  SER A 314     189.636 166.492  -1.893  1.00 16.07      A
C
ATOM   1578  CB  SER A 314     189.229 167.643  -0.984  1.00 17.53      A
C
ATOM   1579  OG  SER A 314     190.261 168.612  -0.972  1.00 25.41      A
O
ATOM   1580  C   SER A 314     189.172 165.168  -1.283  1.00 16.32      A
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ATOM   1582  N   LEU A 315     187.907 164.838  -1.517  1.00 15.55      A
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ATOM   1583  CA  LEU A 315     187.311 163.618  -1.029  1.00 15.03      A
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ATOM   1584  CB  LEU A 315     185.822 163.597  -1.392  1.00 15.51      A
C
ATOM   1585  CG  LEU A 315     184.951 162.599  -0.624  1.00 17.84      A
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ATOM   1586  CD1 LEU A 315     184.877 163.015   0.840  1.00 17.24      A
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ATOM   1587  CD2 LEU A 315     183.555 162.551  -1.222  1.00 15.53      A
C
ATOM   1588  C   LEU A 315     188.031 162.402  -1.626  1.00 15.76      A
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ATOM   1589  O   LEU A 315     188.237 161.399  -0.935  1.00 16.26      A
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ATOM   1590  N   GLY A 316     188.414 162.480  -2.899  1.00 13.03      A
N
ATOM   1591  CA  GLY A 316     189.109 161.357  -3.507  1.00 12.73      A
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ATOM   1592  C   GLY A 316     190.486 161.200  -2.878  1.00 13.41      A
C
ATOM   1593  O   GLY A 316     190.933 160.092  -2.576  1.00 11.78      A
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ATOM   1594  N   VAL A 317     191.167 162.329  -2.702  1.00 12.49      A
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ATOM   1595  CA  VAL A 317     192.481 162.351  -2.089  1.00 11.35      A
C
ATOM   1596  CB  VAL A 317     193.034 163.812  -1.984  1.00 11.65      A
C
ATOM   1597  CG1 VAL A 317     194.231 163.859  -1.079  1.00 10.54      A
C
ATOM   1598  CG2 VAL A 317     193.431 164.323  -3.360  1.00  8.84      A
C
ATOM   1599  C   VAL A 317     192.362 161.759  -0.680  1.00 12.97      A
C
ATOM   1600  O   VAL A 317     193.152 160.887  -0.280  1.00 11.80      A
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ATOM   1601  N   LEU A 318     191.355 162.229   0.052  1.00 10.99      A
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ATOM   1602  CA  LEU A 318     191.097 161.785   1.408  1.00 12.40      A
C
ATOM   1603  CB  LEU A 318     189.958 162.618   2.007  1.00 15.26      A
C
ATOM   1604  CG  LEU A 318     189.652 162.340   3.475  1.00 15.97      A
C
ATOM   1605  CD1 LEU A 318     190.731 162.990   4.377  1.00 14.54      A
C
ATOM   1606  CD2 LEU A 318     188.310 162.873   3.783  1.00 13.89      A
C
ATOM   1607  C   LEU A 318     190.760 160.286   1.527  1.00 12.64      A
C
ATOM   1608  O   LEU A 318     191.232 159.610   2.437  1.00 10.92      A
O
ATOM   1609  N   CYS A 319     189.936 159.778   0.617  1.00 12.91      A
N
ATOM   1610  CA  CYS A 319     189.547 158.372   0.623  1.00 15.63      A
C
ATOM   1611  CB  CYS A 319     188.512 158.092  -0.479  1.00 20.57      A
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ATOM   1612  SG  CYS A 319     187.933 156.363  -0.531  1.00 23.04      A
S
ATOM   1613  C   CYS A 319     190.757 157.490   0.394  1.00 15.66      A
C
ATOM   1614  O   CYS A 319     190.906 156.439   1.025  1.00 15.68      A
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ATOM   1615  N   TYR A 320     191.614 157.922  -0.527  1.00 13.11      A
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ATOM   1616  CA  TYR A 320     192.833 157.194  -0.827  1.00 12.42      A
C
ATOM   1617  CB  TYR A 320     193.560 157.870  -1.999  1.00 12.90      A
C
ATOM   1618  CG  TYR A 320     194.879 157.235  -2.378  1.00 11.79      A
C
ATOM   1619  CD1 TYR A 320     196.014 157.423  -1.594  1.00 11.63      A
C
ATOM   1620  CE1 TYR A 320     197.213 156.803  -1.906  1.00 13.39      A
C
ATOM   1621  CD2 TYR A 320     194.978 156.414  -3.495  1.00 13.02      A
C
ATOM   1622  CE2 TYR A 320     196.167 155.790  -3.822  1.00 14.81      A
C
ATOM   1623  CZ  TYR A 320     197.287 155.980  -3.023  1.00 16.61      A
C
ATOM   1624  OH  TYR A 320     198.459 155.299  -3.325  1.00 14.17      A
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ATOM   1625  C   TYR A 320     193.727 157.138   0.428  1.00 13.58      A
C
ATOM   1626  O   TYR A 320     194.217 156.062   0.797  1.00 12.75      A
O
ATOM   1627  N   GLU A 321     193.922 158.287   1.083  1.00 12.98      A
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ATOM   1628  CA  GLU A 321     194.752 158.359   2.289  1.00 13.87      A
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ATOM   1629  CB  GLU A 321     194.858 159.798   2.815  1.00 15.03      A
C
ATOM   1630  CG  GLU A 321     196.109 160.011   3.685  1.00 22.02      A
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ATOM   1631  CD  GLU A 321     196.204 161.394   4.326  1.00 27.52      A
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ATOM   1632  OE1 GLU A 321     195.889 162.413   3.676  1.00 30.94      A
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ATOM   1633  OE2 GLU A 321     196.621 161.470   5.494  1.00 31.35      A
O
ATOM   1634  C   GLU A 321     194.218 157.470   3.416  1.00 14.01      A
C
ATOM   1635  O   GLU A 321     194.986 156.877   4.166  1.00 14.13      A
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ATOM   1636  N   PHE A 322     192.899 157.384   3.536  1.00 13.55      A
N
ATOM   1637  CA  PHE A 322     192.291 156.568   4.576  1.00 12.09      A
C
ATOM   1638  CB  PHE A 322     190.765 156.710   4.570  1.00  6.70      A
C
ATOM   1639  CG  PHE A 322     190.272 157.975   5.176  1.00  6.79      A
C
ATOM   1640  CD1 PHE A 322     191.144 158.836   5.838  1.00  7.89      A
C
ATOM   1641  CD2 PHE A 322     188.933 158.312   5.106  1.00  8.09      A
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ATOM   1642  CE1 PHE A 322     190.688 160.011   6.416  1.00  6.90      A
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ATOM   1643  CE2 PHE A 322     188.464 159.497   5.689  1.00 10.00      A
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ATOM   1644  CZ  PHE A 322     189.346 160.340   6.345  1.00  8.24      A
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ATOM   1645  C   PHE A 322     192.629 155.107   4.398  1.00 12.56      A
C
ATOM   1646  O   PHE A 322     192.888 154.401   5.375  1.00 14.57      A
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ATOM   1647  N   LEU A 323     192.629 154.663   3.147  1.00 11.23      A
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ATOM   1648  CA  LEU A 323     192.876 153.269   2.830  1.00 10.81      A
C
ATOM   1649  CB  LEU A 323     192.181 152.923   1.510  1.00 11.58      A
C
ATOM   1650  CG  LEU A 323     190.650 152.911   1.467  1.00 11.82      A
C
ATOM   1651  CD1 LEU A 323     190.149 152.693   0.033  1.00  1.00      A
C
ATOM   1652  CD2 LEU A 323     190.158 151.799   2.429  1.00  8.83      A
C
ATOM   1653  C   LEU A 323     194.3   152.888   2.725  1.00 13.31      A
C
ATOM   1654  O   LEU A 323     194.734 151.769   3.072  1.00 13.08      A
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ATOM   1655  N   VAL A 324     195.144 153.832   2.253  1.00 13.79      A
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ATOM   1656  CA  VAL A 324     196.552 153.589   2.028  1.00 13.43      A
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ATOM   1657  CB  VAL A 324     196.958 154.241   0.703  1.00 13.53      A
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ATOM   1658  CG1 VAL A 324     198.387 153.909   0.365  1.00 10.33      A
C
ATOM   1659  CG2 VAL A 324     196.009 153.788  -0.384  1.00 10.31      A
C
ATOM   1660  C   VAL A 324     197.439 154.085   3.153  1.00 15.36      A
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ATOM   1661  O   VAL A 324     198.496 153.525   3.419  1.00 15.10      A
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ATOM   1662  N   GLY A 325     197.019 155.146   3.819  1.00 16.58      A
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ATOM   1663  CA  GLY A 325     197.834 155.647   4.902  1.00 18.98      A
C
ATOM   1664  C   GLY A 325     198.687 156.819   4.459  1.00 22.31      A
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ATOM   1665  O   GLY A 325     199.484 157.330   5.245  1.00 22.91      A
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ATOM   1666  N   LYS A 326     198.556 157.238   3.204  1.00 22.34      A
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ATOM   1667  CA  LYS A 326     199.299 158.399   2.743  1.00 20.73      A
C
ATOM   1668  CB  LYS A 326     200.775 158.057   2.468  1.00 22.54      A
C
ATOM   1669  CG  LYS A 326     201.002 157.016   1.405  1.00 26.76      A
C
ATOM   1670  CD  LYS A 326     202.478 156.728   1.181  1.00 29.37      A
C
ATOM   1671  CE  LYS A 326     202.635 155.634   0.108  1.00 36.99      A
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ATOM   1672  NZ  LYS A 326     204.059 155.235  -0.146  1.00 40.73      A
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ATOM   1673  C   LYS A 326     198.627 158.927   1.496  1.00 18.10      A
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ATOM   1674  O   LYS A 326     198.050 158.173   0.745  1.00 18.75      A
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ATOM   1675  N   PRO A 327     198.657 160.254   1.290  1.00 19.06      A
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ATOM   1676  CD  PRO A 327     199.416 161.265   2.050  1.00 18.18      A
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ATOM   1677  CA  PRO A 327     198.046 160.877   0.111  1.00 16.77      A
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ATOM   1678  CB  PRO A 327     198.349 162.358   0.331  1.00 18.27      A
C
ATOM   1679  CG  PRO A 327     199.652 162.318   0.997  1.00 17.79      A
C
ATOM   1680  C   PRO A 327     198.719 160.334  -1.156  1.00 15.47      A
C
ATOM   1681  O   PRO A 327     199.920 160.074  -1.165  1.00 17.98      A
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ATOM   1682  N   PRO A 328     197.967 160.221  -2.256  1.00 15.81      A
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ATOM   1683  CD  PRO A 328     196.629 160.830  -2.419  1.00 13.52      A
C
ATOM   1684  CA  PRO A 328     198.467 159.699  -3.540  1.00 13.75      A
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ATOM   1685  CB  PRO A 328     197.183 159.511  -4.345  1.00 15.58      A
C
ATOM   1686  CG  PRO A 328     196.384 160.712  -3.922  1.00 15.99      A
C
ATOM   1687  C   PRO A 328     199.517 160.502  -4.312  1.00 14.29      A
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ATOM   1691  CB  PHE A 329     199.880 163.832  -5.357  1.00 11.57      A
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ATOM   1692  CG  PHE A 329     198.677 163.456  -6.171  1.00 10.41      A
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ATOM   1693  CD1 PHE A 329     198.831 162.822  -7.393  1.00  7.22      A
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ATOM   1694  CD2 PHE A 329     197.389 163.646  -5.672  1.00 10.88      A
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ATOM   1695  CE1 PHE A 329     197.722 162.365  -8.117  1.00 11.91      A
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ATOM   1696  CE2 PHE A 329     196.267 163.194  -6.387  1.00  9.29      A
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ATOM   1697  CZ  PHE A 329     196.435 162.548  -7.611  1.00 11.49      A
C
ATOM   1698  C   PHE A 329     201.774 163.073  -3.896  1.00 18.50      A
C
ATOM   1699  O   PHE A 329     202.501 163.999  -4.242  1.00 17.82      A
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ATOM   1700  N   GLU A 330     201.968 162.411  -2.765  1.00 20.96      A
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ATOM   1701  CA  GLU A 330     203.061 162.781  -1.872  1.00 25.68      A
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ATOM   1702  CB  GLU A 330     203.042 161.868  -0.653  1.00 28.63      A
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ATOM   1703  CG  GLU A 330     203.889 162.292   0.527  1.00 35.48      A
C
ATOM   1704  CD  GLU A 330     203.618 161.381   1.725  1.00 40.14      A
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ATOM   1705  OE1 GLU A 330     203.825 161.798   2.890  1.00 43.93      A
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ATOM   1706  OE2 GLU A 330     203.186 160.230   1.490  1.00 43.19      A
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ATOM   1707  C   GLU A 330     204.404 162.666  -2.593  1.00 25.36      A
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ATOM   1708  O   GLU A 330     204.712 161.627  -3.177  1.00 25.32      A
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ATOM   1710  CA  ALA A 331     206.506 163.745  -3.184  1.00 23.23      A
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ATOM   1711  CB  ALA A 331     206.432 164.479  -4.500  1.00 19.73      A
C
ATOM   1712  C   ALA A 331     207.503 164.429  -2.239  1.00 24.76      A
C
ATOM   1713  O   ALA A 331     207.109 165.040  -1.249  1.00 22.52      A
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ATOM   1714  N   ASN A 332     208.794 164.320  -2.542  1.00 27.89      A
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ATOM   1715  CA  ASN A 332     209.822 164.922  -1.692  1.00 30.47      A
C
ATOM   1716  CB  ASN A 332     211.174 164.246  -1.975  1.00 32.87      A
C
ATOM   1717  CG  ASN A 332     211.190 162.794  -1.504  1.00 37.45      A
C
ATOM   1718  OD1 ASN A 332     210.716 162.504  -0.401  1.00 36.73      A
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ATOM   1719  ND2 ASN A 332     211.729 161.883  -2.321  1.00 37.38      A
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ATOM   1720  C   ASN A 332     209.942 166.462  -1.771  1.00 29.91      A
C
ATOM   1721  O   ASN A 332     210.601 167.073  -0.928  1.00 29.72      A
O
ATOM   1722  N   THR A 333     209.303 167.092  -2.754  1.00 27.34      A
N
ATOM   1723  CA  THR A 333     209.369 168.544  -2.881  1.00 25.63      A
C
ATOM   1724  CB  THR A 333     210.411 168.968  -3.919  1.00 27.29      A
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ATOM   1725  OG1 THR A 333     209.862 168.766  -5.232  1.00 25.31      A
O
ATOM   1726  CG2 THR A 333     211.683 168.122  -3.769  1.00 28.40      A
C
ATOM   1727  C   THR A 333     208.021 169.099  -3.341  1.00 24.25      A
C
ATOM   1728  O   THR A 333     207.168 168.355  -3.832  1.00 24.65      A
O
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N
ATOM   1730  CA  TYR A 334     206.610 171.081  -3.584  1.00 24.27      A
C
ATOM   1731  CB  TYR A 334     206.670 172.557  -3.243  1.00 26.40      A
C
ATOM   1732  CG  TYR A 334     206.122 172.899  -1.885  1.00 28.73      A
C
ATOM   1733  CD1 TYR A 334     206.846 172.639  -0.725  1.00 29.53      A
C
ATOM   1734  CE1 TYR A 334     206.322 172.945   0.537  1.00 32.11      A
C
ATOM   1735  CD2 TYR A 334     204.863 173.476  -1.759  1.00 28.50      A
C
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ATOM   1736  CE2 TYR A 334     204.329 173.794  -0.497  1.00 29.43      A
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ATOM   1737  CZ  TYR A 334     205.072 173.518   0.645  1.00 31.88      A
C
ATOM   1738  OH  TYR A 334     204.597 173.783   1.910  1.00 34.80      A
O
ATOM   1739  C   TYR A 334     206.379 170.979  -5.088  1.00 25.01      A
C
ATOM   1740  O   TYR A 334     205.267 170.712  -5.567  1.00 24.09      A
O
ATOM   1741  N   GLN A 335     207.445 171.221  -5.831  1.00 24.15      A
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ATOM   1742  CA  GLN A 335     207.401 171.183  -7.272  1.00 26.26      A
C
ATOM   1743  CB  GLN A 335     208.763 171.616  -7.820  1.00 30.16      A
C
ATOM   1744  CG  GLN A 335     208.690 172.407  -9.123  1.00 37.20      A
C
ATOM   1745  CD  GLN A 335     209.938 173.249  -9.353  1.00 44.29      A
C
ATOM   1746  OE1 GLN A 335     211.075 172.716  -9.361  1.00 45.86      A
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ATOM   1747  NE2 GLN A 335     209.749 174.581  -9.540  1.00 45.65      A
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ATOM   1748  C   GLN A 335     207.014 169.785  -7.766  1.00 24.06      A
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ATOM   1749  O   GLN A 335     206.182 169.643  -8.661  1.00 20.60      A
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ATOM   1750  N   GLU A 336     207.596 168.746  -7.179  1.00 23.21      A
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ATOM   1751  CA  GLU A 336     207.243 167.407  -7.624  1.00 22.61      A
C
ATOM   1752  CB  GLU A 336     208.183 166.360  -7.022  1.00 19.74      A
C
ATOM   1753  CG  GLU A 336     207.807 164.932  -7.350  1.00 27.97      A
C
ATOM   1754  CD  GLU A 336     207.852 164.603  -8.845  1.00 35.28      A
C
ATOM   1755  OE1 GLU A 336     207.231 163.579  -9.236  1.00 38.15      A
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ATOM   1756  OE2 GLU A 336     208.508 165.350  -9.628  1.00 39.74      A
O
ATOM   1757  C   GLU A 336     205.775 167.056  -7.327  1.00 23.14      A
C
ATOM   1758  O   GLU A 336     205.138 166.363  -8.124  1.00 23.03      A
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ATOM   1759  N   THR A 337     205.241 167.517  -6.196  1.00 21.09      A
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ATOM   1760  CA  THR A 337     203.849 167.229  -5.868  1.00 21.21      A
C
ATOM   1761  CB  THR A 337     203.541 167.589  -4.380  1.00 22.66      A
C
ATOM   1762  OG1 THR A 337     204.334 166.744  -3.537  1.00 24.71      A
O
ATOM   1763  CG2 THR A 337     202.072 167.366  -4.030  1.00 16.15      A
C
ATOM   1764  C   THR A 337     202.918 167.944  -6.855  1.00 19.71      A
C
ATOM   1765  O   THR A 337     201.978 167.329  -7.346  1.00 21.88      A
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ATOM   1766  N   TYR A 338     203.191 169.210  -7.171  1.00 17.76      A
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ATOM   1767  CA  TYR A 338     202.404 169.982  -8.151  1.00 17.94      A
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ATOM   1768  CB  TYR A 338     203.051 171.348  -8.416  1.00 19.72      A
C
ATOM   1769  CG  TYR A 338     202.924 172.309  -7.282  1.00 21.47      A
C
ATOM   1770  CD1 TYR A 338     203.927 173.231  -7.014  1.00 26.12      A
C
ATOM   1771  CE1 TYR A 338     203.780 174.172  -6.003  1.00 31.99      A
C
ATOM   1772  CD2 TYR A 338     201.775 172.333  -6.506  1.00 23.72      A
C
ATOM   1773  CE2 TYR A 338     201.609 173.256  -5.498  1.00 28.25      A
C
ATOM   1774  CZ  TYR A 338     202.605 174.184  -5.255  1.00 32.26      A
C
ATOM   1775  OH  TYR A 338     202.398 175.197  -4.343  1.00 37.49      A
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ATOM   1776  C   TYR A 338     202.342 169.248  -9.480  1.00 17.24      A
C
ATOM   1777  O   TYR A 338     201.303 169.202 -10.143  1.00 17.93      A
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ATOM   1778  N   LYS A 339     203.492 168.704  -9.869  1.00 18.06      A
N
ATOM   1779  CA  LYS A 339     203.635 167.967 -11.112  1.00 15.13      A
C
ATOM   1780  CB  LYS A 339     205.087 167.521 -11.318  1.00 15.66      A
C
ATOM   1781  CG  LYS A 339     205.282 166.761 -12.647  1.00 25.11      A
C
ATOM   1782  CD  LYS A 339     206.675 166.164 -12.838  1.00 28.61      A
C
ATOM   1783  CE  LYS A 339     207.736 167.232 -12.973  1.00 30.48      A
C
ATOM   1784  NZ  LYS A 339     209.081 166.590 -13.128  1.00 37.06      A
N
ATOM   1785  C   LYS A 339     202.734 166.747 -11.110  1.00 15.66      A
C
ATOM   1786  O   LYS A 339     201.999 166.520 -12.062  1.00 16.79      A
O
ATOM   1787  N   ARG A 340     202.788 165.963 -10.038  1.00 14.01      A
N
ATOM   1788  CA  ARG A 340     201.980 164.754  -9.941  1.00 17.25      A
C
ATOM   1789  CB  ARG A 340     202.444 163.917  -8.749  1.00 17.92      A
C
ATOM   1790  CG  ARG A 340     203.675 163.112  -9.058  1.00 20.94      A
C
ATOM   1791  CD  ARG A 340     204.273 162.632  -7.805  1.00 26.11      A
C
ATOM   1792  NE  ARG A 340     205.579 162.024  -8.000  1.00 30.74      A
N
ATOM   1793  CZ  ARG A 340     206.247 161.430  -7.014  1.00 34.14      A
C
ATOM   1794  NH1 ARG A 340     205.697 161.387  -5.805  1.00 36.45      A
N
ATOM   1795  NH2 ARG A 340     207.447 160.886  -7.219  1.00 32.82      A
N
ATOM   1796  C   ARG A 340     200.467 164.980  -9.876  1.00 16.32      A
C
ATOM   1797  O   ARG A 340     199.692 164.177 -10.393  1.00 13.54      A
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ATOM   1798  N   ILE A 341     200.052 166.068  -9.242  1.00 16.44      A
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ATOM   1799  CA  ILE A 341     198.637 166.396  -9.147  1.00 15.90      A
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ATOM   1800  CB  ILE A 341     198.425 167.544  -8.133  1.00 14.61      A
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ATOM   1801  CG2 ILE A 341     197.031 168.173  -8.284  1.00 10.21      A
C
ATOM   1802  CG1 ILE A 341     198.636 166.991  -6.722  1.00  9.86      A
C
ATOM   1803  CD1 ILE A 341     198.865 168.066  -5.710  1.00 10.30      A
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ATOM   1804  C   ILE A 341     198.139 166.813 -10.524  1.00 16.94      A
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ATOM   1805  O   ILE A 341     197.099 166.346 -11.003  1.00 15.49      A
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ATOM   1806  N   SER A 342     198.911 167.677 -11.165  1.00 17.49      A
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ATOM   1807  CA  SER A 342     198.556 168.185 -12.479  1.00 19.50      A
C
ATOM   1808  CB  SER A 342     199.638 169.153 -12.927  1.00 19.12      A
C
ATOM   1809  OG  SER A 342     199.178 169.899 -14.023  1.00 28.84      A
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ATOM   1810  C   SER A 342     198.385 167.065 -13.518  1.00 18.65      A
C
ATOM   1811  O   SER A 342     197.544 167.157 -14.414  1.00 17.15      A
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ATOM   1812  N   ARG A 343     199.209 166.027 -13.391  1.00 16.76      A
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ATOM   1813  CA  ARG A 343     199.187 164.881 -14.291  1.00 16.82      A
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ATOM   1814  CB  ARG A 343     200.563 164.214 -14.356  1.00 19.40      A
C
ATOM   1815  CG  ARG A 343     201.744 165.034 -14.873  1.00 20.85      A
C
ATOM   1816  CD  ARG A 343     202.986 164.139 -14.768  1.00 22.63      A
C
ATOM   1817  NE  ARG A 343     204.181 164.667 -15.420  1.00 29.67      A
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ATOM   1818  CZ  ARG A 343     205.296 163.964 -15.619  1.00 29.30      A
C
ATOM   1819  NH1 ARG A 343     205.362 162.702 -15.211  1.00 27.60      A
N
ATOM   1820  NH2 ARG A 343     206.337 164.521 -16.239  1.00 30.90      A
N
ATOM   1821  C   ARG A 343     198.213 163.833 -13.749  1.00 17.95      A
C
ATOM   1822  O   ARG A 343     197.789 162.927 -14.470  1.00 18.61      A
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ATOM   1823  N   VAL A 344     197.880 163.963 -12.465  1.00 16.47      A
N
ATOM   1824  CA  VAL A 344     197.014 163.027 -11.767  1.00 15.15      A
C
ATOM   1825  CB  VAL A 344     195.644 162.882 -12.427  1.00 14.04      A
C
ATOM   1826  CG1 VAL A 344     194.791 161.919 -11.603  1.00 14.73      A
C
ATOM   1827  CG2 VAL A 344     194.949 164.217 -12.503  1.00 14.41      A
C
ATOM   1828  C   VAL A 344     197.751 161.702 -11.847  1.00 19.48      A
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ATOM   1829  O   VAL A 344     197.240 160.697 -12.362  1.00 17.59      A
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ATOM   1830  N   GLU A 345     198.970 161.733 -11.320  1.00 20.63      A
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ATOM   1831  CA  GLU A 345     199.883 160.600 -11.314  1.00 21.68      A
C
ATOM   1832  CB  GLU A 345     201.297 161.116 -11.635  1.00 22.57      A
C
ATOM   1833  CG  GLU A 345     202.291 160.066 -12.115  1.00 29.02      A
C
ATOM   1834  CD  GLU A 345     203.609 160.693 -12.596  1.00 34.43      A
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ATOM   1835  OE1 GLU A 345     203.572 161.826 -13.143  1.00 41.54      A
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ATOM   1836  OE2 GLU A 345     204.677 160.062 -12.448  1.00 34.88      A
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ATOM   1837  C   GLU A 345     199.906 159.839  -9.990  1.00 21.02      A
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ATOM   1838  O   GLU A 345     200.516 160.289  -9.009  1.00 22.86      A
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ATOM   1839  N   PHE A 346     199.260 158.679  -9.953  1.00 20.71      A
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ATOM   1840  CA  PHE A 346     199.268 157.868  -8.730  1.00 20.54      A
C
ATOM   1841  CB  PHE A 346     198.272 158.454  -7.705  1.00 19.53      A
C
ATOM   1842  CG  PHE A 346     196.835 158.138  -8.013  1.00 21.11      A
C
ATOM   1843  CD1 PHE A 346     196.203 157.064  -7.403  1.00 22.02      A
C
ATOM   1844  CD2 PHE A 346     196.130 158.888  -8.936  1.00 18.36      A
C
ATOM   1845  CE1 PHE A 346     194.878 156.744  -7.713  1.00 24.10      A
C
ATOM   1846  CE2 PHE A 346     194.807 158.574  -9.253  1.00 23.07      A
C
ATOM   1847  CZ  PHE A 346     194.181 157.500  -8.640  1.00 22.64      A
C
ATOM   1848  C   PHE A 346     198.893 156.424  -9.065  1.00 19.41      A
C
ATOM   1849  O   PHE A 346     198.376 156.142 -10.153  1.00 21.26      A
O
ATOM   1850  N   THR A 347     199.158 155.512  -8.137  1.00 17.51      A
N
ATOM   1851  CA  THR A 347     198.809 154.113  -8.335  1.00 15.60      A
C
ATOM   1852  CB  THR A 347     200.042 153.259  -8.736  1.00 17.00      A
C
ATOM   1853  OG1 THR A 347     201.113 153.494  -7.812  1.00 20.54      A
O
ATOM   1854  CG2 THR A 347     200.506 153.617 -10.145  1.00 14.88      A
C
ATOM   1855  C   THR A 347     198.245 153.623  -7.026  1.00 14.01      A
C
ATOM   1856  O   THR A 347     198.322 154.324  -6.030  1.00 14.17      A
O
ATOM   1857  N   PHE A 348     197.659 152.434  -7.029  1.00 14.30      A
N
ATOM   1858  CA  PHE A 348     197.097 151.875  -5.809  1.00 15.62      A
C
ATOM   1859  CB  PHE A 348     195.673 151.335  -6.022  1.00 13.71      A
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ATOM   1860  CG  PHE A 348     194.678 152.345  -6.553  1.00 14.90      A
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ATOM   1861  CD1 PHE A 348     194.476 152.496  -7.926  1.00 14.48      A
C
ATOM   1862  CD2 PHE A 348     193.915 153.115  -5.678  1.00 14.25      A
C
ATOM   1863  CE1 PHE A 348     193.520 153.399  -8.421  1.00 13.33      A
C
ATOM   1864  CE2 PHE A 348     192.956 154.020  -6.160  1.00 12.61      A
C
ATOM   1865  CZ  PHE A 348     192.758 154.162  -7.530  1.00 13.12      A
C
ATOM   1866  C   PHE A 348     197.936 150.690  -5.379  1.00 17.39      A
C
ATOM   1867  O   PHE A 348     198.493 149.986  -6.222  1.00 17.79      A
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ATOM   1868  N   PRO A 349     198.077 150.478  -4.060  1.00 19.22      A
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ATOM   1869  CD  PRO A 349     197.716 151.428  -2.984  1.00 20.64      A
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ATOM   1870  CA  PRO A 349     198.843 149.326  -3.550  1.00 18.28      A
C
ATOM   1871  CB  PRO A 349     198.881 149.550  -2.034  1.00 19.47      A
C
ATOM   1872  CG  PRO A 349     198.663 151.042  -1.874  1.00 21.78      A
C
ATOM   1873  C   PRO A 349     197.913 148.144  -3.906  1.00 18.89      A
C
ATOM   1874  O   PRO A 349     196.765 148.365  -4.282  1.00 18.06      A
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ATOM   1875  N   ASP A 350     198.360 146.901  -3.778  1.00 22.60      A
N
ATOM   1876  CA  ASP A 350     197.488 145.780  -4.137  1.00 24.29      A
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ATOM   1877  CB  ASP A 350     198.312 144.494  -4.298  1.00 28.79      A
C
ATOM   1878  CG  ASP A 350     199.378 144.608  -5.404  1.00 33.91      A
C
ATOM   1879  OD1 ASP A 350     200.001 143.575  -5.741  1.00 33.53      A
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ATOM   1880  OD2 ASP A 350     199.591 145.733  -5.928  1.00 35.29      A
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ATOM   1881  C   ASP A 350     196.293 145.489  -3.238  1.00 23.99      A
C
ATOM   1882  O   ASP A 350     195.352 144.835  -3.671  1.00 23.48      A
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ATOM   1883  N   PHE A 351     196.279 145.964  -2.003  1.00 22.20      A
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ATOM   1884  CA  PHE A 351     195.125 145.636  -1.171  1.00 23.75      A
C
ATOM   1885  CB  PHE A 351     195.510 145.662   0.300  1.00 22.72      A
C
ATOM   1886  CG  PHE A 351     196.082 146.956   0.738  1.00 20.40      A
C
ATOM   1887  CD1 PHE A 351     197.451 147.151   0.756  1.00 17.28      A
C
ATOM   1888  CD2 PHE A 351     195.245 147.994   1.111  1.00 19.08      A
C
ATOM   1889  CE1 PHE A 351     197.983 148.379   1.142  1.00 21.72      A
C
ATOM   1890  CE2 PHE A 351     195.761 149.217   1.497  1.00 19.31      A
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ATOM   1891  CZ  PHE A 351     197.128 149.417   1.515  1.00 20.15      A
C
ATOM   1892  C   PHE A 351     193.883 146.509  -1.382  1.00 24.86      A
C
ATOM   1893  O   PHE A 351     192.826 146.215  -0.820  1.00 26.36      A
O
ATOM   1894  N   VAL A 352     193.999 147.575  -2.174  1.00 22.98      A
N
ATOM   1895  CA  VAL A 352     192.845 148.431  -2.428  1.00 22.53      A
C
ATOM   1896  CB  VAL A 352     193.297 149.810  -2.976  1.00 19.91      A
C
ATOM   1897  CG1 VAL A 352     192.105 150.680  -3.293  1.00 15.94      A
C
ATOM   1898  CG2 VAL A 352     194.164 150.489  -1.936  1.00 17.58      A
C
ATOM   1899  C   VAL A 352     191.941 147.702  -3.416  1.00 22.85      A
C
ATOM   1900  O   VAL A 352     192.351 147.406  -4.541  1.00 25.56      A
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ATOM   1901  N   THR A 353     190.722 147.393  -2.985  1.00 20.20      A
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ATOM   1902  CA  THR A 353     189.786 146.668  -3.833  1.00 20.47      A
C
ATOM   1903  CB  THR A 353     188.530 146.264  -3.059  1.00 18.44      A
C
ATOM   1904  OG1 THR A 353     187.777 147.445  -2.740  1.00 19.14      A
O
ATOM   1905  CG2 THR A 353     188.915 145.544  -1.786  1.00 15.00      A
C
ATOM   1906  C   THR A 353     189.331 147.452  -5.049  1.00 23.02      A
C
ATOM   1907  O   THR A 353     189.525 148.665  -5.144  1.00 21.93      A
O
ATOM   1908  N   GLU A 354     188.685 146.733  -5.960  1.00 23.98      A
N
ATOM   1909  CA  GLU A 354     188.175 147.274  -7.208  1.00 25.43      A
C
ATOM   1910  CB  GLU A 354     187.543 146.130  -8.001  1.00 30.21      A
C
ATOM   1911  CG  GLU A 354     186.780 146.540  -9.261  1.00 37.82      A
C
ATOM   1912  CD  GLU A 354     186.031 145.351  -9.890  1.00 41.79      A
C
ATOM   1913  OE1 GLU A 354     185.501 145.472 -11.025  1.00 43.51      A
O
ATOM   1914  OE2 GLU A 354     185.974 144.281  -9.224  1.00 44.80      A
O
ATOM   1915  C   GLU A 354     187.175 148.424  -7.055  1.00 24.34      A
C
ATOM   1916  O   GLU A 354     187.182 149.386  -7.840  1.00 24.85      A
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ATOM   1917  N   GLY A 355     186.298 148.303  -6.065  1.00 20.96      A
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ATOM   1918  CA  GLY A 355     185.289 149.314  -5.842  1.00 13.82      A
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ATOM   1919  C   GLY A 355     185.908 150.595  -5.333  1.00 16.94      A
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ATOM   1920  O   GLY A 355     185.529 151.694  -5.760  1.00 13.60      A
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ATOM   1921  N   ALA A 356     186.868 150.473  -4.425  1.00 15.45      A
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ATOM   1926  N   ARG A 357     188.874 151.611  -5.951  1.00 18.44      A
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ATOM   1927  CA  ARG A 357     189.586 152.184  -7.100  1.00 18.13      A
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ATOM   1928  CB  ARG A 357     190.349 151.113  -7.881  1.00 16.00      A
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ATOM   1929  CG  ARG A 357     191.447 150.447  -7.112  1.00 15.75      A
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ATOM   1930  CD  ARG A 357     192.125 149.414  -7.941  1.00 14.24      A
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N
ATOM   1932  CZ  ARG A 357     194.249 148.203  -7.607  1.00 18.74      A
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ATOM   1933  NH1 ARG A 357     194.553 148.285  -8.898  1.00 21.62      A
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ATOM   1934  NH2 ARG A 357     195.097 147.622  -6.768  1.00 20.49      A
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ATOM   1935  C   ARG A 357     188.627 152.856  -8.062  1.00 17.28      A
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ATOM   1939  CB  ASP A 358     185.267 152.024  -9.389  1.00 21.16      A
C
ATOM   1940  CG  ASP A 358     184.269 152.688 -10.327  1.00 23.93      A
C
ATOM   1941  OD1 ASP A 358     184.508 152.671 -11.559  1.00 29.93      A
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ATOM   1942  OD2 ASP A 358     183.266 153.257  -9.840  1.00 22.82      A
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ATOM   1943  C   ASP A 358     186.081 154.234  -8.611  1.00 17.83      A
C
ATOM   1944  O   ASP A 358     185.996 155.206  -9.348  1.00 20.18      A
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ATOM   1946  CA  LEU A 359     185.389 155.543  -6.680  1.00 15.23      A
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ATOM   1947  CB  LEU A 359     184.873 155.292  -5.250  1.00 13.90      A
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ATOM   1948  CG  LEU A 359     184.459 156.568  -4.482  1.00 15.76      A
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ATOM   1949  CD1 LEU A 359     183.222 157.164  -5.105  1.00 14.16      A
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ATOM   1950  CD2 LEU A 359     184.210 156.266  -3.027  1.00 16.19      A
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ATOM   1951  C   LEU A 359     186.478 156.623  -6.646  1.00 15.38      A
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ATOM   1955  CB  ILE A 360     189.972 156.694  -5.305  1.00 13.18      A
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ATOM   1956  CG2 ILE A 360     191.132 157.645  -5.348  1.00  8.95      A
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ATOM   1957  CG1 ILE A 360     189.613 156.445  -3.843  1.00 11.43      A
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ATOM   1958  CD1 ILE A 360     190.486 155.406  -3.211  1.00 15.13      A
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ATOM   1959  C   ILE A 360     189.126 157.752  -7.457  1.00 18.67      A
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ATOM   1960  O   ILE A 360     189.433 158.935  -7.652  1.00 19.76      A
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ATOM   1961  N   SER A 361     189.099 156.841  -8.427  1.00 17.86      A
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ATOM   1963  CB  SER A 361     189.511 155.952 -10.682  1.00 18.17      A
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ATOM   1964  OG  SER A 361     190.686 155.223 -10.384  1.00 20.30      A
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ATOM   1965  C   SER A 361     188.438 158.163 -10.382  1.00 18.63      A
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ATOM   1966  O   SER A 361     188.805 159.011 -11.209  1.00 19.26      A
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ATOM   1969  CB  ARG A 362     184.740 158.464 -10.227  1.00 18.15      A
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ATOM   1970  CG  ARG A 362     184.389 157.189 -10.948  1.00 21.87      A
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ATOM   1971  CD  ARG A 362     182.950 156.762 -10.710  1.00 24.92      A
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ATOM   1972  NE  ARG A 362     182.669 155.532 -11.449  1.00 31.73      A
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ATOM   1973  CZ  ARG A 362     182.150 155.461 -12.682  1.00 35.25      A
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ATOM   1974  NH1 ARG A 362     181.805 156.557 -13.358  1.00 34.91      A
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ATOM   1975  NH2 ARG A 362     182.052 154.276 -13.281  1.00 35.12      A
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ATOM   1976  C   ARG A 362     186.287 160.332  -9.817  1.00 16.66      A
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ATOM   1977  O   ARG A 362     186.086 161.367 -10.452  1.00 21.59      A
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ATOM   1978  N   LEU A 363     186.602 160.348  -8.527  1.00 15.31      A
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ATOM   1979  CA  LEU A 363     186.726 161.620  -7.814  1.00 15.39      A
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ATOM   1980  CB  LEU A 363     186.758 161.376  -6.295  1.00 13.54      A
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ATOM   1981  CG  LEU A 363     185.452 160.880  -5.638  1.00 14.63      A
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ATOM   1983  CD2 LEU A 363     184.423 162.005  -5.613  1.00  7.80      A
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ATOM   1988  CB  LEU A 364     191.419 161.335  -8.467  1.00 18.29      A
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ATOM   1989  CG  LEU A 364     191.504 161.377  -6.926  1.00 20.11      A
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ATOM   1990  CD1 LEU A 364     192.737 160.607  -6.509  1.00 16.10      A
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ATOM   1991  CD2 LEU A 364     191.576 162.820  -6.413  1.00 16.30      A
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ATOM   1992  C   LEU A 364     190.474 162.393 -10.557  1.00 19.92      A
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ATOM   1993  O   LEU A 364     191.511 162.052 -11.143  1.00 20.12      A
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ATOM   1994  N   LYS A 365     189.450 162.967 -11.169  1.00 19.36      A
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ATOM   1995  CA  LYS A 365     189.461 163.275 -12.581  1.00 19.00      A
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ATOM   1996  CB  LYS A 365     188.039 163.289 -13.117  1.00 22.47      A
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ATOM   1997  CG  LYS A 365     187.417 161.929 -13.243  1.00 23.42      A
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ATOM   1998  CD  LYS A 365     188.039 161.224 -14.400  1.00 23.31      A
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ATOM   2000  NZ  LYS A 365     187.970 159.249 -15.851  1.00 30.35      A
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ATOM   2005  CB  HIS A 366     192.611 166.038 -15.043  1.00 15.66      A
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ATOM   2007  CD2 HIS A 366     194.437 167.877 -14.849  1.00 17.17      A
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ATOM   2008  ND1 HIS A 366     192.763 168.283 -16.194  1.00 19.79      A
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ATOM   2009  CE1 HIS A 366     193.530 169.361 -16.187  1.00 18.47      A
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ATOM   2010  NE2 HIS A 366     194.552 169.141 -15.378  1.00 18.20      A
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ATOM   2011  C   HIS A 366     190.493 167.186 -14.291  1.00 17.88      A
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ATOM   2012  O   HIS A 366     190.553 168.334 -13.864  1.00 14.94      A
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ATOM   2014  CA  ASN A 367     188.436 167.676 -15.490  1.00 22.11      A
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ATOM   2017  OD1 ASN A 367     185.990 168.718 -16.827  1.00 34.30      A
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ATOM   2018  ND2 ASN A 367     187.209 168.611 -18.688  1.00 31.42      A
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ATOM   2019  C   ASN A 367     187.348 167.721 -14.412  1.00 22.00      A
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ATOM   2020  O   ASN A 367     186.644 166.739 -14.198  1.00 21.37      A
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ATOM   2024  CB  PRO A 368     186.292 170.571 -12.377  1.00 23.08      A
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ATOM   2025  CG  PRO A 368     187.705 170.942 -12.864  1.00 19.70      A
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ATOM   2026  C   PRO A 368     184.755 168.638 -13.047  1.00 22.70      A
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ATOM   2027  O   PRO A 368     184.016 168.091 -12.209  1.00 21.09      A
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ATOM   2028  N   SER A 369     184.386 168.865 -14.303  1.00 21.10      A
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ATOM   2029  CA  SER A 369     183.068 168.492 -14.818  1.00 25.15      A
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ATOM   2030  CB  SER A 369     182.919 168.982 -16.263  1.00 25.61      A
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ATOM   2031  OG  SER A 369     183.115 170.391 -16.341  1.00 37.93      A
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ATOM   2032  C   SER A 369     182.809 166.986 -14.785  1.00 23.28      A
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ATOM   2033  O   SER A 369     181.685 166.555 -14.591  1.00 26.91      A
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ATOM   2034  N   GLN A 370     183.848 166.196 -14.995  1.00 20.71      A
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ATOM   2035  CA  GLN A 370     183.744 164.749 -15.009  1.00 21.53      A
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ATOM   2036  CB  GLN A 370     184.922 164.172 -15.785  1.00 24.23      A
C
ATOM   2037  CG  GLN A 370     184.674 164.178 -17.279  1.00 31.18      A
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ATOM   2038  CD  GLN A 370     185.948 164.183 -18.045  1.00 38.83      A
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ATOM   2039  OE1 GLN A 370     186.879 163.380 -17.767  1.00 41.58      A
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ATOM   2040  NE2 GLN A 370     186.033 165.098 -19.038  1.00 43.83      A
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ATOM   2041  C   GLN A 370     183.688 164.073 -13.665  1.00 20.69      A
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ATOM   2042  O   GLN A 370     183.444 162.864 -13.600  1.00 19.42      A
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ATOM   2043  N   ARG A 371     183.940 164.804 -12.585  1.00 18.88      A
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ATOM   2049  CZ  ARG A 371     188.440 167.951  -9.938  1.00 14.14      A
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ATOM   2055  CD  PRO A 372     183.165 162.051  -9.512  1.00 23.75      A
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ATOM   2056  CA  PRO A 372     180.757 162.663  -9.653  1.00 21.80      A
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ATOM   2057  CB  PRO A 372     180.923 161.269  -9.007  1.00 22.29      A
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ATOM   2058  CG  PRO A 372     182.365 161.227  -8.548  1.00 22.92      A
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ATOM   2059  C   PRO A 372     180.160 163.726  -8.739  1.00 21.72      A
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ATOM   2060  O   PRO A 372     180.875 164.579  -8.217  1.00 23.11      A
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ATOM   2062  CA  MET A 373     178.153 164.668  -7.731  1.00 19.68      A
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ATOM   2063  CB  MET A 373     176.674 164.841  -8.137  1.00 25.32      A
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ATOM   2064  CG  MET A 373     176.470 165.598  -9.397  1.00 29.58      A
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ATOM   2065  SD  MET A 373     177.274 167.224  -9.216  1.00 44.08      A
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ATOM   2066  CE  MET A 373     175.850 168.314  -8.571  1.00 34.35      A
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ATOM   2067  C   MET A 373     178.231 163.942  -6.368  1.00 18.77      A
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ATOM   2068  O   MET A 373     178.518 162.750  -6.337  1.00 14.31      A
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ATOM   2070  CA  LEU A 374     178.041 163.984  -3.959  1.00 17.05      A
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ATOM   2071  CB  LEU A 374     177.959 165.010  -2.820  1.00 15.61      A
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ATOM   2072  CG  LEU A 374     179.224 165.888  -2.751  1.00 17.98      A
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ATOM   2073  CD1 LEU A 374     178.940 167.269  -2.145  1.00  8.94      A
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ATOM   2074  CD2 LEU A 374     180.290 165.125  -1.973  1.00 12.26      A
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ATOM   2076  O   LEU A 374     177.122 161.885  -3.201  1.00 19.21      A
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ATOM   2077  N   ARG A 375     175.804 163.167  -4.504  1.00 18.78      A
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ATOM   2078  CA  ARG A 375     174.657 162.248  -4.510  1.00 20.13      A
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ATOM   2080  C   ARG A 375     175.033 160.942  -5.178  1.00 21.00      A
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ATOM   2081  O   ARG A 375     174.457 159.916  -4.909  1.00 21.05      A
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ATOM   2082  N   GLU A 376     175.970 161.009  -6.106  1.00 23.11      A
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ATOM   2083  CA  GLU A 376     176.419 159.788  -6.763  1.00 23.55      A
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ATOM   2084  CB  GLU A 376     177.142 160.139  -8.053  1.00 24.82      A
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ATOM   2085  CG  GLU A 376     176.400 161.110  -8.977  1.00 32.25      A
C
ATOM   2086  CD  GLU A 376     177.239 161.561 -10.206  1.00 34.95      A
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ATOM   2087  OE1 GLU A 376     177.030 162.670 -10.770  1.00 37.06      A
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ATOM   2088  OE2 GLU A 376     178.110 160.783 -10.630  1.00 37.87      A
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ATOM   2089  C   GLU A 376     177.380 158.962  -5.852  1.00 23.36      A
C
ATOM   2090  O   GLU A 376     177.448 157.712  -5.874  1.00 25.32      A
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ATOM   2091  N   VAL A 377     178.204 159.683  -5.113  1.00 20.65      A
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ATOM   2092  CA  VAL A 377     179.168 159.065  -4.241  1.00 19.06      A
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ATOM   2093  CB  VAL A 377     180.021 160.117  -3.550  1.00 20.25      A
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ATOM   2094  CG1 VAL A 377     180.772 159.513  -2.415  1.00 14.07      A
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ATOM   2095  CG2 VAL A 377     180.949 160.762  -4.587  1.00 16.78      A
C
ATOM   2096  C   VAL A 377     178.386 158.284  -3.229  1.00 20.23      A
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ATOM   2097  O   VAL A 377     178.647 157.099  -3.037  1.00 20.59      A
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ATOM   2100  CB  LEU A 378     175.514 159.346  -1.107  1.00 19.33      A
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ATOM   2103  CD2 LEU A 378     175.575 161.610   0.073  1.00 20.05      A
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ATOM   2116  CA  HIS A 380     178.278 154.301  -5.145  1.00 20.63      A
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ATOM   2117  CB  HIS A 380     179.683 154.909  -4.995  1.00 15.41      A
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ATOM   2122  NE2 HIS A 380     182.042 153.399  -7.372  1.00 15.37      A
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ATOM   2124  O   HIS A 380     178.129 152.774  -3.293  1.00 21.40      A
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ATOM   2125  N   PRO A 381     178.231 151.843  -5.333  1.00 21.11      A
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ATOM   2128  CB  PRO A 381     178.512 149.635  -6.139  1.00 23.24      A
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ATOM   2134  CB  TRP A 382     182.667 150.885  -3.160  1.00 16.26      A
C
ATOM   2135  CG  TRP A 382     183.757 150.595  -2.180  1.00 17.75      A
C
ATOM   2136  CD2 TRP A 382     184.370 151.524  -1.271  1.00 17.24      A
C
ATOM   2137  CE2 TRP A 382     185.366 150.816  -0.559  1.00 16.47      A
C
ATOM   2138  CE3 TRP A 382     184.165 152.882  -0.983  1.00 17.55      A
C
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ATOM   2139  CD1 TRP A 382     184.389 149.398  -1.986  1.00 14.76      A
C
ATOM   2140  NE1 TRP A 382     185.358 149.524  -1.022  1.00 16.65      A
N
ATOM   2141  CZ2 TRP A 382     186.168 151.422   0.421  1.00 15.85      A
C
ATOM   2142  CZ3 TRP A 382     184.965 153.487  -0.002  1.00 19.06      A
C
ATOM   2143  CH2 TRP A 382     185.951 152.754   0.687  1.00 17.35      A
C
ATOM   2144  C   TRP A 382     180.898 151.042  -1.431  1.00 18.11      A
C
ATOM   2145  O   TRP A 382     181.045 150.467  -0.352  1.00 19.08      A
O
ATOM   2146  N   ILE A 383     180.391 152.266  -1.533  1.00 18.03      A
N
ATOM   2147  CA  ILE A 383     179.963 153.003  -0.354  1.00 17.34      A
C
ATOM   2148  CB  ILE A 383     179.585 154.460  -0.709  1.00 15.70      A
C
ATOM   2149  CG2 ILE A 383     178.985 155.178   0.495  1.00 13.48      A
C
ATOM   2150  CG1 ILE A 383     180.841 155.212  -1.132  1.00  8.79      A
C
ATOM   2151  CD1 ILE A 383     181.809 155.455   0.019  1.00 11.19      A
C
ATOM   2152  C   ILE A 383     178.790 152.312   0.324  1.00 19.72      A
C
ATOM   2153  O   ILE A 383     178.851 152.044   1.523  1.00 21.11      A
O
ATOM   2154  N   THR A 384     177.739 151.994  -0.428  1.00 18.67      A
N
ATOM   2155  CA  THR A 384     176.585 151.336   0.180  1.00 21.04      A
C
ATOM   2156  CB  THR A 384     175.352 151.287  -0.784  1.00 22.27      A
C
ATOM   2157  OG1 THR A 384     175.657 150.457  -1.912  1.00 23.10      A
O
ATOM   2158  CG2 THR A 384     174.969 152.706  -1.271  1.00 15.14      A
C
ATOM   2159  C   THR A 384     176.868 149.921   0.721  1.00 20.77      A
C
ATOM   2160  O   THR A 384     176.220 149.496   1.683  1.00 24.40      A
O
ATOM   2161  N   ALA A 385     177.835 149.206   0.138  1.00 18.85      A
N
ATOM   2162  CA  ALA A 385     178.195 147.848   0.598  1.00 16.58      A
C
ATOM   2163  CB  ALA A 385     178.996 147.119  -0.481  1.00  8.89      A
C
ATOM   2164  C   ALA A 385     179.021 147.877   1.890  1.00 19.30      A
C
ATOM   2165  O   ALA A 385     178.987 146.950   2.699  1.00 17.69      A
O
ATOM   2166  N   ASN A 386     179.748 148.966   2.104  1.00 23.78      A
N
ATOM   2167  CA  ASN A 386     180.614 149.059   3.274  1.00 24.44      A
C
ATOM   2168  CB  ASN A 386     182.039 149.240   2.783  1.00 22.82      A
C
ATOM   2169  CG  ASN A 386     182.509 148.051   1.997  1.00 22.92      A
C
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ATOM   2170  OD1 ASN A 386     182.581 146.947   2.539  1.00 23.56      A
O
ATOM   2171  ND2 ASN A 386     182.807 148.251   0.706  1.00 20.68      A
N
ATOM   2172  C   ASN A 386     180.305 150.133   4.291  1.00 25.32      A
C
ATOM   2173  O   ASN A 386     180.891 150.175   5.366  1.00 25.70      A
O
ATOM   2174  N   SER A 387     179.385 151.009   3.950  1.00 28.67      A
N
ATOM   2175  CA  SER A 387     179.063 152.111   4.823  1.00 30.65      A
C
ATOM   2176  CB  SER A 387     178.507 153.232   3.955  1.00 29.51      A
C
ATOM   2177  OG  SER A 387     178.208 154.364   4.724  1.00 35.78      A
O
ATOM   2178  C   SER A 387     178.063 151.687   5.890  1.00 32.67      A
C
ATOM   2179  O   SER A 387     177.162 150.889   5.535  1.00 35.02      A
O
ATOM   2180  OXT SER A 387     178.173 152.164   7.055  1.00 35.90      A
O
ATOM   2181  CB  SER B   7     187.273 195.899  10.921  1.00 30.72      B
C
ATOM   2182  OG  SER B   7     185.919 195.490  11.062  1.00 28.92      B
O
ATOM   2183  C   SER B   7     187.728 193.792  12.227  1.00 32.69      B
C
ATOM   2184  O   SER B   7     187.932 192.918  11.331  1.00 33.35      B
O
ATOM   2185  N   SER B   7     189.583 195.368  11.576  1.00 34.34      B
N
ATOM   2186  CA  SER B   7     188.150 195.268  12.001  1.00 32.37      B
C
ATOM   2187  N   TYR B   8     187.139 193.527  13.402  1.00 28.10      B
N
ATOM   2188  CA  TYR B   8     186.671 192.188  13.775  1.00 25.10      B
C
ATOM   2189  CB  TYR B   8     187.465 191.681  14.999  1.00 22.64      B
C
ATOM   2190  CG  TYR B   8     188.962 191.579  14.731  1.00 22.03      B
C
ATOM   2191  CD1 TYR B   8     189.806 192.667  14.982  1.00 19.79      B
C
ATOM   2192  CE1 TYR B   8     191.153 192.623  14.642  1.00 19.33      B
C
ATOM   2193  CD2 TYR B   8     189.524 190.435  14.128  1.00 18.09      B
C
ATOM   2194  CE2 TYR B   8     190.881 190.391  13.775  1.00 18.91      B
C
ATOM   2195  CZ  TYR B   8     191.686 191.488  14.038  1.00 20.94      B
C
ATOM   2196  OH  TYR B   8     193.020 191.444  13.712  1.00 23.31      B
O
ATOM   2197  C   TYR B   8     185.151 192.143  14.045  1.00 24.33      B
C
ATOM   2198  O   TYR B   8     184.677 191.422  14.936  1.00 23.49      B
O
ATOM   2199  N   SER B   9     184.410 192.931  13.263  1.00 24.49      B
N
ATOM   2200  CA  SER B   9     182.945 193.017  13.314  1.00 24.46      B
C
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ATOM   2201  CB  SER B   9     182.455 194.444  13.006  1.00 23.56      B
C
ATOM   2202  OG  SER B   9     182.756 195.336  14.059  1.00 29.98      B
O
ATOM   2203  C   SER B   9     182.426 192.085  12.229  1.00 22.36      B
C
ATOM   2204  O   SER B   9     182.469 192.408  11.035  1.00 22.10      B
O
ATOM   2205  N   TYR B  10     181.926 190.938  12.653  1.00 20.97      B
N
ATOM   2206  CA  TYR B  10     181.434 189.932  11.728  1.00 21.80      B
C
ATOM   2207  CB  TYR B  10     182.099 188.582  12.063  1.00 21.23      B
C
ATOM   2208  CG  TYR B  10     183.618 188.617  12.082  1.00 23.30      B
C
ATOM   2209  CD1 TYR B  10     184.345 187.694  12.836  1.00 24.95      B
C
ATOM   2210  CE1 TYR B  10     185.744 187.683  12.816  1.00 25.40      B
C
ATOM   2211  CD2 TYR B  10     184.331 189.542  11.311  1.00 23.55      B
C
ATOM   2212  CE2 TYR B  10     185.725 189.541  11.285  1.00 24.34      B
C
ATOM   2213  CZ  TYR B  10     186.421 188.600  12.036  1.00 26.19      B
C
ATOM   2214  OH  TYR B  10     187.800 188.526  11.956  1.00 31.92      B
O
ATOM   2215  C   TYR B  10     179.918 189.807  11.832  1.00 21.84      B
C
ATOM   2216  O   TYR B  10     179.334 190.098  12.872  1.00 22.91      B
O
ATOM   2217  N   ASP B  11     179.283 189.372  10.754  1.00 19.80      B
N
ATOM   2218  CA  ASP B  11     177.842 189.173  10.751  1.00 19.63      B
C
ATOM   2219  CB  ASP B  11     177.308 189.274   9.310  1.00 21.09      B
C
ATOM   2220  CG  ASP B  11     175.778 189.141   9.217  1.00 23.91      B
C
ATOM   2221  OD1 ASP B  11     175.093 188.957  10.256  1.00 24.67      B
O
ATOM   2222  OD2 ASP B  11     175.264 189.221   8.077  1.00 22.90      B
O
ATOM   2223  C   ASP B  11     177.653 187.756  11.297  1.00 19.67      B
C
ATOM   2224  O   ASP B  11     177.383 186.820  10.565  1.00 20.37      B
O
ATOM   2225  N   ALA B  12     177.844 187.593  12.590  1.00 19.26      B
N
ATOM   2226  CA  ALA B  12     177.696 186.285  13.174  1.00 19.72      B
C
ATOM   2227  CB  ALA B  12     178.993 185.498  13.013  1.00 20.60      B
C
ATOM   2228  C   ALA B  12     177.337 186.502  14.640  1.00 20.60      B
C
ATOM   2229  O   ALA B  12     177.450 187.632  15.149  1.00 20.41      B
O
ATOM   2230  N   PRO B  13     176.918 185.448  15.350  1.00 20.13      B
N
ATOM   2231  CD  PRO B  13     176.769 184.055  14.907  1.00 17.56      B
C
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ATOM   2232  CA  PRO B  13     176.545 185.608  16.761  1.00 16.88       B
C
ATOM   2233  CB  PRO B  13     175.959 184.246  17.137  1.00 16.25       B
C
ATOM   2234  CG  PRO B  13     175.670 183.563  15.811  1.00 18.64       B
C
ATOM   2235  C   PRO B  13     177.663 186.014  17.728  1.00 17.09       B
C
ATOM   2236  O   PRO B  13     178.797 185.573  17.590  1.00 17.90       B
O
ATOM   2237  N   SER B  14     177.334 186.839  18.720  1.00 17.14       B
N
ATOM   2238  CA  SER B  14     178.294 187.258  19.739  1.00 20.00       B
C
ATOM   2239  CB  SER B  14     179.094 188.499  19.294  1.00 19.42       B
C
ATOM   2240  OG  SER B  14     178.288 189.384  18.544  1.00 30.47       B
O
ATOM   2241  C   SER B  14     177.587 187.518  21.069  1.00 18.32       B
C
ATOM   2242  O   SER B  14     178.199 187.968  22.056  1.00 14.51       B
O
ATOM   2243  N   ASP B  15     176.297 187.215  21.076  1.00 18.48       B
N
ATOM   2244  CA  ASP B  15     175.445 187.376  22.248  1.00 23.79       B
C
ATOM   2245  CB  ASP B  15     173.991 187.526  21.783  1.00 30.49       B
C
ATOM   2246  CG  ASP B  15     173.676 188.932  21.226  1.00 39.83       B
C
ATOM   2247  OD1 ASP B  15     174.558 189.605  20.616  1.00 44.43       B
O
ATOM   2248  OD2 ASP B  15     172.510 189.378  21.401  1.00 45.45       B
O
ATOM   2249  C   ASP B  15     175.569 186.172  23.199  1.00 21.79       B
C
ATOM   2250  O   ASP B  15     175.594 185.035  22.754  1.00 22.39       B
O
ATOM   2251  N   PHE B  16     175.660 186.432  24.500  1.00 21.47       B
N
ATOM   2252  CA  PHE B  16     175.756 185.373  25.514  1.00 22.21       B
C
ATOM   2253  CB  PHE B  16     175.700 185.993  26.930  1.00 19.46       B
C
ATOM   2254  CG  PHE B  16     175.637 184.978  28.025  1.00 18.34       B
C
ATOM   2255  CD1 PHE B  16     176.789 184.362  28.491  1.00 18.98       B
C
ATOM   2256  CD2 PHE B  16     174.417 184.569  28.528  1.00 15.51       B
C
ATOM   2257  CE1 PHE B  16     176.716 183.339  29.435  1.00 18.59       B
C
ATOM   2258  CE2 PHE B  16     174.340 183.552  29.469  1.00 15.01       B
C
ATOM   2259  CZ  PHE B  16     175.488 182.939  29.921  1.00 15.05       B
C
ATOM   2260  C   PHE B  16     174.542 184.448  25.301  1.00 21.16       B
C
ATOM   2261  O   PHE B  16     173.442 184.938  25.058  1.00 21.78       B
O
ATOM   2262  N   ILE B  17     174.739 183.135  25.370  1.00 19.97       B
N
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ATOM   2263  CA  ILE B  17     173.652 182.163  25.182  1.00 20.86      B
C
ATOM   2264  CB  ILE B  17     173.965 181.144  24.009  1.00 21.47      B
C
ATOM   2265  CG2 ILE B  17     172.988 179.964  24.011  1.00 11.76      B
C
ATOM   2266  CG1 ILE B  17     173.957 181.844  22.654  1.00 16.04      B
C
ATOM   2267  CD1 ILE B  17     174.760 181.051  21.631  1.00 18.42      B
C
ATOM   2268  C   ILE B  17     173.478 181.318  26.439  1.00 21.56      B
C
ATOM   2269  O   ILE B  17     174.462 180.965  27.086  1.00 23.11      B
O
ATOM   2270  N   ASN B  18     172.227 181.002  26.778  1.00 24.87      B
N
ATOM   2271  CA  ASN B  18     171.893 180.143  27.928  1.00 26.79      B
C
ATOM   2272  CB  ASN B  18     170.485 180.437  28.427  1.00 26.34      B
C
ATOM   2273  CG  ASN B  18     170.052 179.482  29.543  1.00 30.28      B
C
ATOM   2274  OD1 ASN B  18     170.753 178.519  29.870  1.00 30.01      B
O
ATOM   2275  ND2 ASN B  18     168.893 179.747  30.125  1.00 28.50      B
N
ATOM   2276  C   ASN B  18     171.911 178.718  27.373  1.00 28.06      B
C
ATOM   2277  O   ASN B  18     170.947 178.305  26.737  1.00 31.09      B
O
ATOM   2278  N   PHE B  19     172.969 177.950  27.616  1.00 30.32      B
N
ATOM   2279  CA  PHE B  19     173.027 176.599  27.050  1.00 32.46      B
C
ATOM   2280  CB  PHE B  19     174.460 176.061  27.076  1.00 27.50      B
C
ATOM   2281  CG  PHE B  19     175.430 176.837  26.214  1.00 22.59      B
C
ATOM   2282  CD1 PHE B  19     176.332 177.737  26.785  1.00 20.42      B
C
ATOM   2283  CD2 PHE B  19     175.426 176.682  24.831  1.00 21.89      B
C
ATOM   2284  CE1 PHE B  19     177.223 178.454  25.989  1.00 19.77      B
C
ATOM   2285  CE2 PHE B  19     176.312 177.398  24.021  1.00 18.13      B
C
ATOM   2286  CZ  PHE B  19     177.206 178.291  24.605  1.00 19.50      B
C
ATOM   2287  C   PHE B  19     172.086 175.529  27.618  1.00 36.90      B
C
ATOM   2288  O   PHE B  19     172.063 174.397  27.124  1.00 41.31      B
O
ATOM   2289  N   SER B  20     171.317 175.844  28.646  1.00 41.32      B
N
ATOM   2290  CA  SER B  20     170.402 174.824  29.142  1.00 46.46      B
C
ATOM   2291  CB  SER B  20     170.317 174.921  30.652  1.00 47.60      B
C
ATOM   2292  OG  SER B  20     170.456 176.275  31.032  1.00 49.62      B
O
ATOM   2293  C   SER B  20     169.029 175.021  28.496  1.00 48.43      B
C
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ATOM   2294  O   SER B  20     168.337 174.060  28.170  1.00 50.43      B
O
ATOM   2295  N   SER B  21     168.645 176.275  28.286  1.00 50.08      B
N
ATOM   2296  CA  SER B  21     167.349 176.574  27.676  1.00 50.65      B
C
ATOM   2297  CB  SER B  21     166.742 177.810  28.317  1.00 49.82      B
C
ATOM   2298  OG  SER B  21     167.467 178.945  27.866  1.00 50.01      B
O
ATOM   2299  C   SER B  21     167.581 176.880  26.204  1.00 51.89      B
C
ATOM   2300  O   SER B  21     166.843 176.336  25.325  1.00 51.53      B
O
ATOM   2301  OXT SER B  21     168.482 177.716  25.953  1.00 53.54      B
O
ATOM   2302  CB  ASN C  30     165.336 177.781  10.155  1.00 41.18      C
C
ATOM   2303  CG  ASN C  30     164.486 178.568   9.178  1.00 46.58      C
C
ATOM   2304  OD1 ASN C  30     164.828 179.693   8.808  1.00 49.62      C
O
ATOM   2305  ND2 ASN C  30     163.363 177.973   8.740  1.00 49.11      C
N
ATOM   2306  C   ASN C  30     167.301 179.381  10.314  1.00 36.00      C
C
ATOM   2307  O   ASN C  30     167.202 179.731   9.143  1.00 34.36      C
O
ATOM   2308  N   ASN C  30     165.267 179.744  11.676  1.00 37.72      C
N
ATOM   2309  CA  ASN C  30     166.154 178.688  11.078  1.00 38.33      C
C
ATOM   2310  N   ILE C  31     168.406 179.537  11.026  1.00 32.89      C
N
ATOM   2311  CA  ILE C  31     169.605 180.229  10.589  1.00 28.57      C
C
ATOM   2312  CB  ILE C  31     170.635 180.011  11.676  1.00 31.08      C
C
ATOM   2313  CG2 ILE C  31     171.873 180.840  11.426  1.00 30.71      C
C
ATOM   2314  CG1 ILE C  31     169.991 180.405  13.012  1.00 34.10      C
C
ATOM   2315  CD1 ILE C  31     169.738 181.909  13.147  1.00 41.37      C
C
ATOM   2316  C   ILE C  31     170.254 180.041   9.214  1.00 25.67      C
C
ATOM   2317  O   ILE C  31     170.816 180.996   8.677  1.00 20.90      C
O
ATOM   2318  N   ASP C  32     170.188 178.856   8.623  1.00 23.52      C
N
ATOM   2319  CA  ASP C  32     170.872 178.678   7.351  1.00 24.02      C
C
ATOM   2320  CB  ASP C  32     171.126 177.197   7.086  1.00 27.28      C
C
ATOM   2321  CG  ASP C  32     169.858 176.423   6.805  1.00 32.74      C
C
ATOM   2322  OD1 ASP C  32     168.852 177.009   6.338  1.00 36.15      C
O
ATOM   2323  OD2 ASP C  32     169.884 175.202   7.039  1.00 33.71      C
O
ATOM   2324  C   ASP C  32     170.289 179.324   6.104  1.00 23.19      C
C
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ATOM   2325  O   ASP C  32     170.804 179.126   5.001  1.00 22.55      C
O
ATOM   2326  N   SER C  33     169.223 180.090   6.271  1.00 21.46      C
N
ATOM   2327  CA  SER C  33     168.608 180.781   5.136  1.00 22.57      C
C
ATOM   2328  CB  SER C  33     167.205 181.244   5.499  1.00 23.28      C
C
ATOM   2329  OG  SER C  33     166.326 180.142   5.639  1.00 33.59      C
O
ATOM   2330  C   SER C  33     169.448 182.002   4.805  1.00 19.49      C
C
ATOM   2331  O   SER C  33     169.273 182.639   3.770  1.00 20.33      C
O
ATOM   2332  N   TRP C  34     170.344 182.330   5.728  1.00 18.04      C
N
ATOM   2333  CA  TRP C  34     171.254 183.466   5.621  1.00 16.02      C
C
ATOM   2334  CB  TRP C  34     172.234 183.422   6.792  1.00 15.82      C
C
ATOM   2335  CG  TRP C  34     173.240 184.531   6.836  1.00 15.40      C
C
ATOM   2336  CD2 TRP C  34     174.599 184.462   6.404  1.00 13.15      C
C
ATOM   2337  CE2 TRP C  34     175.180 185.735   6.640  1.00 14.42      C
C
ATOM   2338  CE3 TRP C  34     175.387 183.451   5.843  1.00 10.87      C
C
ATOM   2339  CD1 TRP C  34     173.052 185.801   7.302  1.00 13.49      C
C
ATOM   2340  NE1 TRP C  34     174.212 186.530   7.189  1.00 11.42      C
N
ATOM   2341  CZ2 TRP C  34     176.523 186.024   6.330  1.00 14.91      C
C
ATOM   2342  CZ3 TRP C  34     176.727 183.738   5.538  1.00 12.26      C
C
ATOM   2343  CH2 TRP C  34     177.278 185.016   5.785  1.00 10.61      C
C
ATOM   2344  C   TRP C  34     172.022 183.499   4.299  1.00 15.62      C
C
ATOM   2345  O   TRP C  34     172.251 184.579   3.735  1.00 16.88      C
O
ATOM   2346  N   PHE C  35     172.435 182.324   3.819  1.00 13.45      C
N
ATOM   2347  CA  PHE C  35     173.191 182.222   2.567  1.00 12.33      C
C
ATOM   2348  CB  PHE C  35     173.739 180.801   2.344  1.00  8.78      C
C
ATOM   2349  CG  PHE C  35     174.597 180.304   3.456  1.00  9.30      C
C
ATOM   2350  CD1 PHE C  35     174.042 179.566   4.495  1.00  9.43      C
C
ATOM   2351  CD2 PHE C  35     175.960 180.610   3.500  1.00  9.38      C
C
ATOM   2352  CE1 PHE C  35     174.822 179.141   5.565  1.00  6.69      C
C
ATOM   2353  CE2 PHE C  35     176.749 180.190   4.569  1.00  8.62      C
C
ATOM   2354  CZ  PHE C  35     176.174 179.455   5.602  1.00 10.55      C
C
ATOM   2355  C   PHE C  35     172.367 182.623   1.351  1.00 13.51      C
C
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ATOM   2356  O   PHE C  35     172.779 183.502   0.597  1.00 13.63      C
O
ATOM   2357  N   ALA C  36     171.207 181.997   1.153  1.00 14.52      C
N
ATOM   2358  CA  ALA C  36     170.392 182.349  -0.008  1.00 18.05      C
C
ATOM   2359  CB  ALA C  36     169.246 181.349  -0.209  1.00 13.28      C
C
ATOM   2360  C   ALA C  36     169.844 183.775   0.103  1.00 18.08      C
C
ATOM   2361  O   ALA C  36     169.797 184.500  -0.899  1.00 20.25      C
O
ATOM   2362  N   GLU C  37     169.458 184.192   1.307  1.00 18.61      C
N
ATOM   2363  CA  GLU C  37     168.905 185.536   1.505  1.00 21.91      C
C
ATOM   2364  CB  GLU C  37     168.391 185.686   2.933  1.00 22.41      C
C
ATOM   2365  CG  GLU C  37     167.103 184.901   3.240  1.00 24.75      C
C
ATOM   2366  CD  GLU C  37     166.619 185.133   4.681  1.00 30.55      C
C
ATOM   2367  OE1 GLU C  37     167.473 185.511   5.529  1.00 31.00      C
O
ATOM   2368  OE2 GLU C  37     165.414 184.932   4.976  1.00 30.11      C
O
ATOM   2369  C   GLU C  37     169.913 186.649   1.194  1.00 22.74      C
C
ATOM   2370  O   GLU C  37     169.561 187.754   0.791  1.00 22.40      C
O
ATOM   2371  N   LYS C  38     171.181 186.332   1.375  1.00 25.80      C
N
ATOM   2372  CA  LYS C  38     172.269 187.252   1.114  1.00 24.79      C
C
ATOM   2373  CB  LYS C  38     173.438 186.831   1.982  1.00 27.15      C
C
ATOM   2374  CG  LYS C  38     174.708 187.488   1.649  1.00 30.16      C
C
ATOM   2375  CD  LYS C  38     175.776 187.057   2.622  1.00 31.96      C
C
ATOM   2376  CE  LYS C  38     177.007 187.927   2.391  1.00 35.28      C
C
ATOM   2377  NZ  LYS C  38     178.028 187.735   3.456  1.00 40.31      C
N
ATOM   2378  C   LYS C  38     172.625 187.194  -0.373  1.00 25.05      C
C
ATOM   2379  O   LYS C  38     173.062 188.177  -0.969  1.00 23.54      C
O
ATOM   2380  N   ALA C  39     172.418 186.032  -0.975  1.00 23.76      C
N
ATOM   2381  CA  ALA C  39     172.687 185.849  -2.400  1.00 23.35      C
C
ATOM   2382  CB  ALA C  39     172.656 184.343  -2.762  1.00 20.98      C
C
ATOM   2383  C   ALA C  39     171.642 186.576  -3.245  1.00 24.77      C
C
ATOM   2384  O   ALA C  39     171.950 187.112  -4.318  1.00 24.28      C
O
ATOM   2385  N   ASN C  40     170.403 186.592  -2.754  1.00 23.38      C
N
ATOM   2386  CA  ASN C  40     169.306 187.210  -3.480  1.00 23.68      C
C
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ATOM   2387  CB  ASN C  40     167.993 186.526  -3.137  1.00 18.03      C
C
ATOM   2388  CG  ASN C  40     168.024 185.035  -3.395  1.00 17.89      C
C
ATOM   2389  OD1 ASN C  40     168.646 184.553  -4.351  1.00 18.06      C
O
ATOM   2390  ND2 ASN C  40     167.325 184.287  -2.545  1.00 16.76      C
N
ATOM   2391  C   ASN C  40     169.122 188.701  -3.279  1.00 25.17      C
C
ATOM   2392  O   ASN C  40     168.413 189.332  -4.052  1.00 27.11      C
O
ATOM   2393  N   LEU C  41     169.731 189.268  -2.246  1.00 26.95      C
N
ATOM   2394  CA  LEU C  41     169.600 190.709  -1.965  1.00 29.31      C
C
ATOM   2395  CB  LEU C  41     170.380 191.047  -0.705  1.00 29.88      C
C
ATOM   2396  CG  LEU C  41     169.816 192.308  -0.057  1.00 30.53      C
C
ATOM   2397  CD1 LEU C  41     168.319 192.148   0.221  1.00 30.41      C
C
ATOM   2398  CD2 LEU C  41     170.580 192.558   1.209  1.00 29.64      C
C
ATOM   2399  C   LEU C  41     170.091 191.589  -3.120  1.00 29.84      C
C
ATOM   2400  O   LEU C  41     171.051 191.230  -3.787  1.00 30.13      C
O
ATOM   2401  N   GLU C  42     169.487 192.763  -3.312  1.00 32.17      C
N
ATOM   2402  CA  GLU C  42     169.851 193.627  -4.439  1.00 35.33      C
C
ATOM   2403  CB  GLU C  42     168.583 193.847  -5.286  1.00 33.50      C
C
ATOM   2404  CG  GLU C  42     167.819 192.560  -5.616  1.00 32.30      C
C
ATOM   2405  CD  GLU C  42     166.473 192.784  -6.334  1.00 34.80      C
C
ATOM   2406  OE1 GLU C  42     165.892 193.892  -6.241  1.00 34.22      C
O
ATOM   2407  OE2 GLU C  42     165.980 191.829  -6.987  1.00 33.99      C
O
ATOM   2408  C   GLU C  42     170.537 194.977  -4.190  1.00 37.36      C
C
ATOM   2409  O   GLU C  42     170.487 195.539  -3.109  1.00 38.22      C
O
ATOM   2410  N   ASN C  43     171.220 195.457  -5.221  1.00 43.15      C
N
ATOM   2411  CA  ASN C  43     171.863 196.790  -5.266  1.00 48.74      C
C
ATOM   2412  CB  ASN C  43     172.611 197.184  -3.967  1.00 48.84      C
C
ATOM   2413  CG  ASN C  43     173.769 196.255  -3.632  1.00 50.97      C
C
ATOM   2414  OD1 ASN C  43     173.749 195.054  -3.970  1.00 50.34      C
O
ATOM   2415  ND2 ASN C  43     174.793 196.804  -2.939  1.00 51.10      C
N
ATOM   2416  C   ASN C  43     172.809 196.704  -6.455  1.00 52.67      C
C
ATOM   2417  O   ASN C  43     172.493 197.379  -7.493  1.00 54.34      C
O
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ATOM   2418  OXT ASN C  43     173.808 195.931  -6.344  1.00 55.98      C
O
ATOM   2419  PB  ADP S 531     193.788 175.824  12.432  1.00 20.87      S
P
ATOM   2420  O1B ADP S 531     193.884 176.352  13.792  1.00 32.28      S
O
ATOM   2421  O2B ADP S 531     193.566 176.837  11.394  1.00 26.12      S
O
ATOM   2422  O3B ADP S 531     194.979 174.908  12.132  1.00 31.89      S
O
ATOM   2423  PA  ADP S 531     191.748 174.063  13.545  1.00 18.35      S
P
ATOM   2424  O1A ADP S 531     190.611 174.901  14.032  1.00 26.99      S
O
ATOM   2425  O2A ADP S 531     191.357 172.755  12.954  1.00 26.80      S
O
ATOM   2426  O3A ADP S 531     192.532 174.874  12.450  1.00 28.14      S
O
ATOM   2427  O5* ADP S 531     192.642 173.906  14.839  1.00 22.21      S
O
ATOM   2428  C5* ADP S 531     193.768 172.965  14.869  1.00 20.71      S
C
ATOM   2429  C4* ADP S 531     193.594 171.623  15.640  1.00 17.30      S
C
ATOM   2430  O4* ADP S 531     192.923 171.842  16.897  1.00 18.08      S
O
ATOM   2431  C3* ADP S 531     192.751 170.494  14.997  1.00 17.80      S
C
ATOM   2432  O3* ADP S 531     193.561 169.824  14.038  1.00 18.78      S
O
ATOM   2433  C2* ADP S 531     192.369 169.659  16.218  1.00 19.78      S
C
ATOM   2434  O2* ADP S 531     193.423 168.749  16.615  1.00 19.10      S
O
ATOM   2435  C1* ADP S 531     192.152 170.704  17.312  1.00 18.01      S
C
ATOM   2436  N9  ADP S 531     190.711 171.169  17.445  1.00 18.12      S
N
ATOM   2437  C8  ADP S 531     190.169 172.237  16.808  1.00 20.72      S
C
ATOM   2438  N7  ADP S 531     188.877 172.431  17.108  1.00 19.94      S
N
ATOM   2439  C5  ADP S 531     188.596 171.408  17.961  1.00 15.87      S
C
ATOM   2440  C6  ADP S 531     187.377 171.071  18.652  1.00 14.49      S
C
ATOM   2441  N6  ADP S 531     186.260 171.696  18.563  1.00  9.66      S
N
ATOM   2442  N1  ADP S 531     187.474 169.935  19.454  1.00 13.01      S
N
ATOM   2443  C2  ADP S 531     188.642 169.198  19.595  1.00 14.56      S
C
ATOM   2444  N3  ADP S 531     189.773 169.512  18.982  1.00 17.25      S
N
ATOM   2445  C4  ADP S 531     189.716 170.610  18.162  1.00 16.09      S
C
ATOM   2446  MG  MG  X   1     192.801 173.013  10.897  1.00 18.98      X
MG+2
ATOM   2447  MG  MG  X   2     192.933 178.461  10.215  1.00 21.17      X
MG+2
ATOM   2448  MG  MG  X   3     174.135 172.090  -6.081  1.00 37.43      X
MG+2
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ATOM   2449  S   SO4 Y   1     175.520 167.060  -4.810  1.00 40.27      Y
S
ATOM   2450  O1  SO4 Y   1     175.005 168.134  -3.755  1.00 40.61      Y
O
ATOM   2451  O2  SO4 Y   1     176.918 167.395  -5.118  1.00 40.85      Y
O
ATOM   2452  O3  SO4 Y   1     175.333 165.874  -4.319  1.00 45.29      Y
O
ATOM   2453  O4  SO4 Y   1     174.705 167.387  -6.003  1.00 46.53      Y
O
ATOM   2454  S   SO4 Y   2     196.317 160.442  22.149  1.00 52.91      Y
S
ATOM   2455  O1  SO4 Y   2     194.902 160.702  22.904  1.00 53.25      Y
O
ATOM   2456  O2  SO4 Y   2     197.156 161.615  22.484  1.00 52.23      Y
O
ATOM   2457  O3  SO4 Y   2     196.808 159.261  22.506  1.00 50.45      Y
O
ATOM   2458  O4  SO4 Y   2     195.932 160.567  20.717  1.00 53.17      Y
O
ATOM   2459  S   SO4 Y   3     184.237 187.281  -0.473  1.00 69.64      Y
S
ATOM   2460  O1  SO4 Y   3     182.905 188.209  -0.613  1.00 70.60      Y
O
ATOM   2461  O2  SO4 Y   3     185.274 188.143   0.172  1.00 70.08      Y
O
ATOM   2462  O3  SO4 Y   3     183.925 186.181   0.170  1.00 69.68      Y
O
ATOM   2463  O4  SO4 Y   3     184.641 187.119  -1.915  1.00 70.92      Y
O
ATOM   2464  OH2 WAT W   1     179.030 185.642  -6.293  1.00  8.84      W
O
ATOM   2465  OH2 WAT W   2     194.313 179.202  -8.444  1.00 16.79      W
O
ATOM   2466  OH2 WAT W   3     192.921 180.168   8.084  1.00 30.46      W
O
ATOM   2467  OH2 WAT W   4     187.994 175.656   4.804  1.00 16.00      W
O
ATOM   2468  OH2 WAT W   5     178.455 169.305  -5.499  1.00 13.87      W
O
ATOM   2469  OH2 WAT W   6     197.111 180.066  22.244  1.00 15.19      W
O
ATOM   2470  OH2 WAT W   7     180.414 171.384  22.814  1.00  8.30      W
O
ATOM   2471  OH2 WAT W   8     188.179 184.543  -6.390  1.00 10.24      W
O
ATOM   2472  OH2 WAT W   9     188.183 181.649   3.509  1.00 23.15      W
O
ATOM   2473  OH2 WAT W  10     185.065 157.114  14.496  1.00 16.39      W
O
ATOM   2474  OH2 WAT W  11     192.854 158.543  18.441  1.00 20.42      W
O
ATOM   2475  OH2 WAT W  12     194.144 171.703  11.618  1.00 13.61      W
O
ATOM   2476  OH2 WAT W  13     194.572 183.197  -8.077  1.00 36.64      W
O
ATOM   2477  OH2 WAT W  14     198.254 147.344  -7.377  1.00 23.99      W
O
ATOM   2478  OH2 WAT W  15     174.141 170.073  -2.678  1.00 18.36      W
O
ATOM   2479  OH2 WAT W  16     197.136 162.247   7.860  1.00 20.24      W
O
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ATOM   2480  OH2 WAT W  17     178.742 175.122  -2.821  1.00 12.41       W
O
ATOM   2481  OH2 WAT W  18     200.365 168.406   2.165  1.00  9.98       W
O
ATOM   2482  OH2 WAT W  19     168.522 176.594   9.704  1.00 27.47       W
O
ATOM   2483  OH2 WAT W  20     193.215 179.995  11.973  1.00 17.15       W
O
ATOM   2484  OH2 WAT W  21     188.165 173.468  14.493  1.00 18.83       W
O
ATOM   2485  OH2 WAT W  22     178.977 189.493   5.006  1.00 25.99       W
O
ATOM   2486  OH2 WAT W  23     194.904 178.835  14.332  1.00  9.84       W
O
ATOM   2487  OH2 WAT W  24     172.594 187.824  25.336  1.00 22.88       W
O
ATOM   2488  OH2 WAT W  25     186.612 173.366  -9.877  1.00 19.22       W
O
ATOM   2489  OH2 WAT W  26     176.840 183.702  20.193  1.00 22.57       W
O
ATOM   2490  OH2 WAT W  27     176.801 160.388  11.646  1.00 15.90       W
O
ATOM   2491  OH2 WAT W  28     178.487 174.788  11.702  1.00 18.10       W
O
ATOM   2492  OH2 WAT W  29     181.155 186.952  32.619  1.00 32.00       W
O
ATOM   2493  OH2 WAT W  30     209.304 163.564 -16.281  1.00 27.44       W
O
ATOM   2494  OH2 WAT W  31     203.827 165.930  -0.838  1.00 16.37       W
O
ATOM   2495  OH2 WAT W  32     183.937 190.638  21.333  1.00 17.02       W
O
ATOM   2496  OH2 WAT W  33     190.362 181.451   8.363  1.00 23.84       W
O
ATOM   2497  OH2 WAT W  34     201.524 183.136  11.412  1.00 27.78       W
O
ATOM   2498  OH2 WAT W  35     176.401 172.283  12.285  1.00 22.44       W
O
ATOM   2499  OH2 WAT W  36     191.486 178.801  -8.556  1.00 14.47       W
O
ATOM   2500  OH2 WAT W  37     193.706 178.975  16.555  1.00 28.73       W
O
ATOM   2501  OH2 WAT W  38     200.711 191.015   5.492  1.00 22.39       W
O
ATOM   2502  OH2 WAT W  39     198.698 163.980  -2.087  1.00 16.88       W
O
ATOM   2503  OH2 WAT W  40     186.096 174.714  13.402  1.00 14.25       W
O
ATOM   2504  OH2 WAT W  41     189.561 189.228  27.405  1.00 21.42       W
O
ATOM   2505  OH2 WAT W  42     185.742 175.020 -12.633  1.00 32.61       W
O
ATOM   2506  OH2 WAT W  43     189.284 166.218  21.436  1.00 18.57       W
O
ATOM   2507  OH2 WAT W  44     189.806 150.396  10.582  1.00 17.00       W
O
ATOM   2508  OH2 WAT W  45     182.606 183.843   1.498  1.00 23.82       W
O
ATOM   2509  OH2 WAT W  46     203.088 159.272  -4.093  1.00 20.75       W
O
ATOM   2510  OH2 WAT W  47     197.775 190.097  18.980  1.00 22.00       W
O
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ATOM   2511  OH2 WAT W  48     193.113 164.352  18.292  1.00 18.52      W
O
ATOM   2512  OH2 WAT W  49     188.303 192.170   8.139  1.00 29.33      W
O
ATOM   2513  OH2 WAT W  50     178.988 188.073  29.292  1.00 22.03      W
O
ATOM   2514  OH2 WAT W  51     179.041 176.835  -4.879  1.00 28.93      W
O
ATOM   2515  OH2 WAT W  52     177.094 169.275  14.745  1.00 17.83      W
O
ATOM   2516  OH2 WAT W  53     173.359 158.848   5.717  1.00 26.69      W
O
ATOM   2517  OH2 WAT W  54     184.713 145.517  -1.099  1.00 25.66      W
O
ATOM   2518  OH2 WAT W  55     197.989 162.673  24.709  1.00 31.35      W
O
ATOM   2519  OH2 WAT W  56     190.279 149.132  -0.366  1.00 23.37      W
O
ATOM   2520  OH2 WAT W  57     175.195 156.308   1.515  1.00 25.31      W
O
ATOM   2521  OH2 WAT W  58     189.320 149.244  12.871  1.00 39.74      W
O
ATOM   2522  OH2 WAT W  59     191.345 160.562  17.366  1.00 19.61      W
O
ATOM   2523  OH2 WAT W  60     209.300 189.438  10.191  1.00 32.59      W
O
ATOM   2524  OH2 WAT W  61     176.961 195.154  23.343  1.00 26.84      W
O
ATOM   2525  OH2 WAT W  62     194.908 178.479  10.038  1.00 12.42      W
O
ATOM   2526  OH2 WAT W  63     192.932 176.681   8.727  1.00 17.49      W
O
ATOM   2527  OH2 WAT W  64     191.151 178.650  10.287  1.00 25.58      W
O
ATOM   2528  OH2 WAT W  65     182.000 183.023 -13.348  1.00 15.88      W
O
ATOM   2529  OH2 WAT W  66     174.844 179.377  29.234  1.00 21.85      W
O
ATOM   2530  OH2 WAT W  67     192.666 150.025   4.037  1.00 24.70      W
O
ATOM   2531  OH2 WAT W  68     191.227 167.117  19.848  1.00 27.52      W
O
ATOM   2532  OH2 WAT W  69     195.798 166.787  -4.678  1.00 16.05      W
O
ATOM   2533  OH2 WAT W  70     188.683 164.953  24.250  1.00 16.65      W
O
ATOM   2534  OH2 WAT W  71     202.921 187.953   5.807  1.00 25.48      W
O
ATOM   2535  OH2 WAT W  72     173.656 180.838  -1.296  1.00 19.16      W
O
ATOM   2536  OH2 WAT W  73     178.223 170.722  21.753  1.00 28.96      W
O
ATOM   2537  OH2 WAT W  74     200.047 185.273   4.691  1.00 36.63      W
O
ATOM   2538  OH2 WAT W  75     199.421 160.492  21.694  1.00 54.41      W
O
ATOM   2539  OH2 WAT W  76     174.343 151.575  -4.090  1.00 24.22      W
O
ATOM   2540  OH2 WAT W  77     199.217 156.232   8.084  1.00 24.50      W
O
ATOM   2541  OH2 WAT W  78     186.693 195.451  15.184  1.00 30.28      W
O
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ATOM   2542  OH2 WAT W  79     204.072 167.051 -16.474  1.00 30.81       W
O
ATOM   2543  OH2 WAT W  80     189.729 170.883  13.071  1.00 24.00       W
O
ATOM   2544  OH2 WAT W  81     193.562 167.033  18.576  1.00 34.40       W
O
ATOM   2545  OH2 WAT W  82     188.055 177.150 -16.174  1.00 39.31       W
O
ATOM   2546  OH2 WAT W  83     209.167 161.801  -3.764  1.00 29.76       W
O
ATOM   2547  OH2 WAT W  84     189.954 187.203  -3.104  1.00 30.21       W
O
ATOM   2548  OH2 WAT W  85     166.356 175.210   9.226  1.00 35.64       W
O
ATOM   2549  OH2 WAT W  86     209.038 162.643 -13.951  1.00 29.71       W
O
ATOM   2550  OH2 WAT W  87     179.913 164.861  20.417  1.00 23.03       W
O
ATOM   2551  OH2 WAT W  88     176.985 177.272  13.711  1.00 28.39       W
O
ATOM   2552  OH2 WAT W  89     197.775 160.663  10.355  1.00 30.90       W
O
ATOM   2553  OH2 WAT W  90     180.418 156.423 -15.983  1.00 38.69       W
O
ATOM   2554  OH2 WAT W  91     197.603 165.048   7.104  1.00 39.85       W
O
ATOM   2555  OH2 WAT W  92     201.038 146.684  -3.627  1.00 28.72       W
O
ATOM   2556  OH2 WAT W  93     191.798 173.307  -1.526  1.00 20.55       W
O
ATOM   2557  OH2 WAT W  94     195.433 186.638   2.426  1.00 32.36       W
O
ATOM   2558  OH2 WAT W  95     185.689 149.073  10.194  1.00 32.44       W
O
ATOM   2559  OH2 WAT W  96     181.725 186.361   4.468  1.00 44.13       W
O
ATOM   2560  OH2 WAT W  97     190.638 181.376   1.418  1.00 40.50       W
O
ATOM   2561  OH2 WAT W  98     203.221 164.983   2.765  1.00 30.78       W
O
ATOM   2562  OH2 WAT W  99     191.430 148.459   1.931  1.00 29.87       W
O
ATOM   2563  OH2 WAT W 100     172.186 178.856  -0.480  1.00 35.57       W
O
ATOM   2564  OH2 WAT W 101     195.541 178.234   1.979  1.00 25.17       W
O
ATOM   2565  OH2 WAT W 102     170.598 187.029  21.078  1.00 24.60       W
O
ATOM   2566  OH2 WAT W 103     175.607 172.274  -8.036  1.00 36.47       W
O
ATOM   2567  OH2 WAT W 104     168.429 188.864  -6.367  1.00 22.94       W
O
ATOM   2568  OH2 WAT W 105     186.340 190.812  24.666  1.00 32.99       W
O
ATOM   2569  OH2 WAT W 106     201.816 192.555   4.023  1.00 28.31       W
O
ATOM   2570  OH2 WAT W 107     202.504 159.814  -7.441  1.00 22.58       W
O
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O
ATOM   2572  OH2 WAT W 109     175.457 179.403  15.662  1.00 39.35       W
O
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ATOM   2573  OH2 WAT W 110     196.564 193.700   7.818  1.00 32.38       W
O
ATOM   2574  OH2 WAT W 111     173.232 181.808  -8.349  1.00 19.06       W
O
ATOM   2575  OH2 WAT W 112     182.827 187.517  -4.364  1.00 45.61       W
O
ATOM   2576  OH2 WAT W 113     189.838 194.231   7.217  1.00 42.16       W
O
ATOM   2577  OH2 WAT W 114     191.170 159.628 -12.340  1.00 35.35       W
O
ATOM   2578  OH2 WAT W 115     191.207 184.866  -0.535  1.00 34.38       W
O
ATOM   2579  OH2 WAT W 116     183.572 197.288  15.706  1.00 39.58       W
O
ATOM   2580  OH2 WAT W 117     199.841 150.695  13.176  1.00 35.40       W
O
ATOM   2581  OH2 WAT W 118     174.316 180.622  18.227  1.00 29.36       W
O
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O
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O
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O
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O
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O
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O
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O
ATOM   2589  OH2 WAT W 126     172.799 187.052  31.328  1.00 38.58       W
O
ATOM   2590  OH2 WAT W 127     173.867 181.212  14.618  1.00 28.93       W
O
ATOM   2591  OH2 WAT W 128     169.850 183.554   9.734  1.00 31.19       W
O
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O
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O
ATOM   2594  OH2 WAT W 131     195.036 155.601  22.286  1.00 43.08       W
O
ATOM   2595  OH2 WAT W 132     188.136 149.463 -10.689  1.00 31.69       W
O
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O
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O
ATOM   2598  OH2 WAT W 135     173.141 166.101   3.246  1.00 37.73       W
O
ATOM   2599  OH2 WAT W 136     196.411 181.887  24.452  1.00 31.18       W
O
ATOM   2600  OH2 WAT W 137     166.875 190.046  -8.389  1.00 35.44       W
O
ATOM   2601  OH2 WAT W 138     168.310 173.985   5.026  1.00 36.83       W
O
ATOM   2602  OH2 WAT W 139     191.553 162.337 -15.173  1.00 30.34       W
O
ATOM   2603  OH2 WAT W 140     196.789 179.956   0.077  1.00 34.96       W
O
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ATOM   2604  OH2 WAT W 141     204.362 177.082  -3.998  1.00 42.74       W
O
ATOM   2605  OH2 WAT W 142     178.237 157.118  15.427  1.00 37.51       W
O
ATOM   2606  OH2 WAT W 143     180.703 166.918  18.919  1.00 22.25       W
O
ATOM   2607  OH2 WAT W 144     190.076 196.775  13.865  1.00 38.81       W
O
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Claims

1. A crystal of phosphorylated human Aurora-A kinase fragment comprising amino acid residues 122-403 complexed with amino acid residues 1-43 of human TPX2, wherein said crystal diffracts to at least 3 angstrom resolution and has a crystal stability within 5% of its unit cell dimensions.

2. The crystal according to claim 1, having the coordinates as listed in Table B.

3. The crystal according to claim 1 or 2, said crystal belonging to the orthorhombic space group $P2_12_12_1$ and having the unit cell dimensions in angstroms: a = 59.63 ± 5%, b = 81.72 ± 5%, c = 70.38 ± 5%.

4. The crystal according to any one of claims 1 to 3, having a Aurora-A ligand binding site defined by the structure coordinates of Aurora-A amino acids Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 according to Table B.

5. A molecule or molecular complexe comprising at least a part of the ligand binding site defined by structure coordinates of Aurora-A amino acids Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 according to Table B, or a mutant or homologue thereof.

6. A machine-readable data storage medium comprising a data storage material encoded with machine readable data, wherein the data is defined by the structure coordinates of phosphorylated human Aurora-A kinase complexed with amino acid residues 1-43 of human TPX2 according to Table B or a homologue of said complex, wherein said homologue comprises backbone atoms that have a root mean square deviation from the backbone atoms of the complex of not more than 3.0 A.

7. A binding site in Aurora-A, or a homologue or mutant thereof, for an AR modulator in which a portion of said ligand is in van der Walls contact or hydrogen bonding contact with any portion or all of residues Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A according toTable B.

8. The binding site according to claim 7, wherein the homologue or mutant has 25%-95% identity to residues Q127, W128, R126, L159, F157, E170, L169, V206, Y199,

H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A according toTable B.

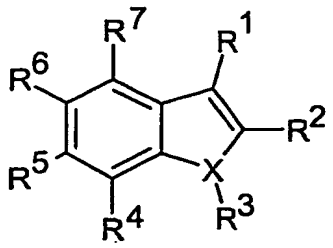
9. A method for identifying a compound that modulates Aurora-A kinase activity, the method comprising any combination of steps of :
a) modeling test compounds that fit spatially into the Aurora-A binding site as defined by structure coordinates according to Table B;
b) using said structure coordinates or binding site as set forth in claim 7 to identify structural and chemical features;
c) employing identified structural or chemical features to design or select compounds as potential Aurora-A modulators;
d) employing the three-dimensional structural model or the ligand binding site to design or select compounds as potential Aurora-A modulators;
e) synthesizing the potential Aurora-A modulators;
f) screening the potential Aurora-A modulators in an assay characterized by binding of a test compound to the Aurora-A; and
g) modifying or replacing one or more amino acids from Aurora-A selected from the group consisting of Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A according to Table B.

10. An Aurora-A modulator identified by the method of claim 9.

11. An allosteric inhibitor of Aurora-A, at least a portion of which binds with any portion or all of residues Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A according to Table B.

12. The allosteric inhibitor of claim 11, wherein binding is van der Walls contact or hydrogen bonding contact.

13. Indole and indene derivatives of formula (I)



(I)

wherein

R^1 represents hydrogen, alkylene-NHR^8, alkylene-OR^8, or alkylene-SR^8;

R^2 represents hydrogen, alkylene-NHR^8, alkylene-OR^8, or alkylene-SR^8;

R^3 represents hydrogen, alkyl, alkylene-R^9, alkenylene-R^9, alkynylene-R^9, or arylene-R^9;

R^4 represents hydrogen;

R^5 represents hydrogen, alkyl, OR^{10}, NHR^{10}, SR^{10}, alkylene-R^{10}, alkenylene-R^{10}, alkynylene-R^{10}, or arylene-R^{10};

R^6 represents hydrogen, alkyl, OR^{10}, NHR^{10}, SR^{10}, alkylene-R^{10}, alkenylene-R^{10}, alkynylene-R^{10}, or arylene-R^{10};

R^7 represents hydrogen;

R^8 represents hydrogen, CO-alkyl, $(aa)_m asp(aa)_n$, $(aa)_m glu(aa)_n$, or $(aa)_m cys(aa)_n$;

R^9 represents NH-alkyl, $N(alkyl)_2$, $N^+(alkyl)_3$, aryl, or heteroaryl;

R^{10} represents hydrogen, aryl, or substituted aryl;

X represents a nitrogen atom or CH;

aa represents an amino acid radical; and

n is zero or an integer of 1 to 10;

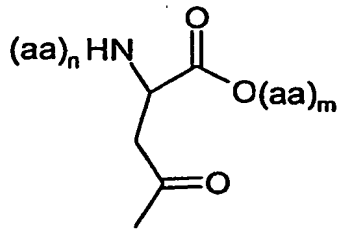
m is zero or an integer of 1 to 10,

provided that R^1 and R^2 are not both hydrogen and that R^5 and R^6 are not both hydrogen,

and optical isomers, physiologically acceptable salts and prodrugs thereof.

14. The compound according to claim 13, wherein one of residues R^1 and R^2, preferably R^2, is hydrogen and the other, preferably R^1, represents alkylene-NHR^8.

15. The compound according to claim 13 or 14, wherein R^8 is a radical of the formula (II)



(II)

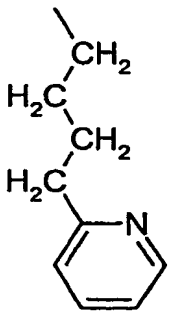
wherein

aa represents an amino acid radical;

n is zero or an integer of 1 to 10; and

m is zero or an integer of 1 to 10.

16. The compound according to any one of claims 13 to 15, wherein R^3 is a radical of the formula (IV)



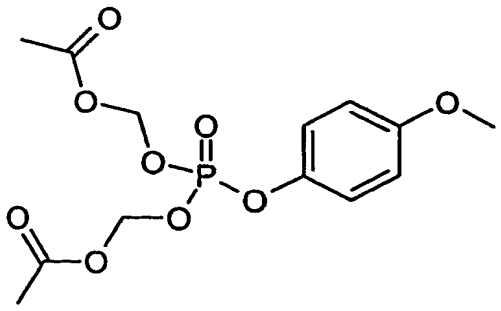
(IV)

17. The compound according to any one of claims 13 to 16, wherein R^5 and/or R^6 represent OR^{10}, wherein R^{10} is defined as in claim 13.

18. The compound according to any one of claims 13 to 17, wherein R^{10} is aryl which may be substituted with 1, 2 or 3 substituents independently selected from the group consisting of hydroxy $-OPO_3H_2$, $-CH_2PO_3H_2$, $-CF_2PO_3H_2$, -COOH, $-CH(COOH)_2$, $-OPO_3(R^{11})_2$, $-CH_2OPO_3(R^{11})_2$, $-CF_2PO_3(R^{11})_2$, $-COOR^{11}$, and $-CH(COOR^{11})_2$, wherein R^{11} is a radical that is cleavable *in vivo*.

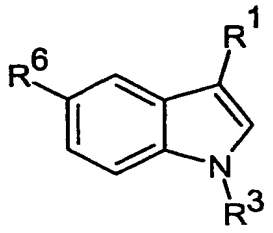
19. The compound according to claim 18, wherein R^{11} represents alkyl, CH_2OCO-alkyl, and C_2H_4-S-CO-alkyl.

20. The compound according to any one of claims 13 to 19, wherein R^5 and/or R^6 are/is the radical of formula (V)



(V)

21. The compound according to claim 13, having the formula (Ia)

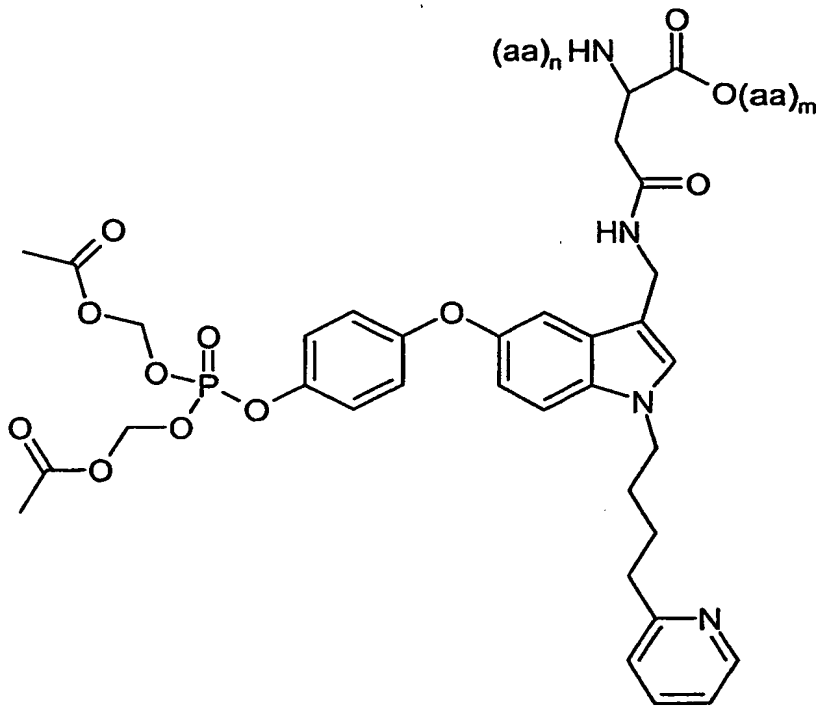


(Ia)

wherein

R^1, R^3 and R^6 are defined as in any one of claims 13 to 20.

22. The indole derivative of formula (1)



1

wherein

aa, n and m are defined as in claim 13,

and optical isomers and physiologically acceptable salts thereof.

23. The Aurora-A modulator of claim 10, the allosteric inhibitor of claims 11 or 12, or the indole or indene derivative of any one of claims 13 to 22 for use in therapy.

24. Pharmaceutical composition, comprising at least one Aurora-A modulator of claim 10, at least one allosteric inhibitor of claims 11 or 12, or at least one indole or indene

derivative of any one of claims 13 to 22, optionally in combination with a pharmaceutically acceptable excipient.

25. The use of an Aurora-A modulator of claim 10, of an allosteric inhibitor of claims 11 or 12, or of an indole or indene derivative of any one of claims 13 to 22 in the manufacture of a medicament for treating cancer.

26. The use according to claim 25, wherein the cancer is a breast or colon carcinoma.

Abstract

The present invention relates to crystals of phosphorylated Aurora-A kinase fragment alone and in complex with a ligand, amino acid residues 1-43 of human TPX2. This invention also relates to methods for designing and selecting ligands, in particular allosteric inhibitors of Aurora-A, that bind to the Aurora-A kinase and their use. Further, the present invention relates to certain indene and indole derivatives.The present invention relates to crystals of phosphorylated Aurora-A kinase alone and in complex with a ligand, amino acid residues 1-43 of human TPX2. This invention also relates to methods for designing and selecting ligands that bind to the Aurora-A kinase and their use. Further, the present invention relates to certain indene and indole derivatives.

Fig. 1

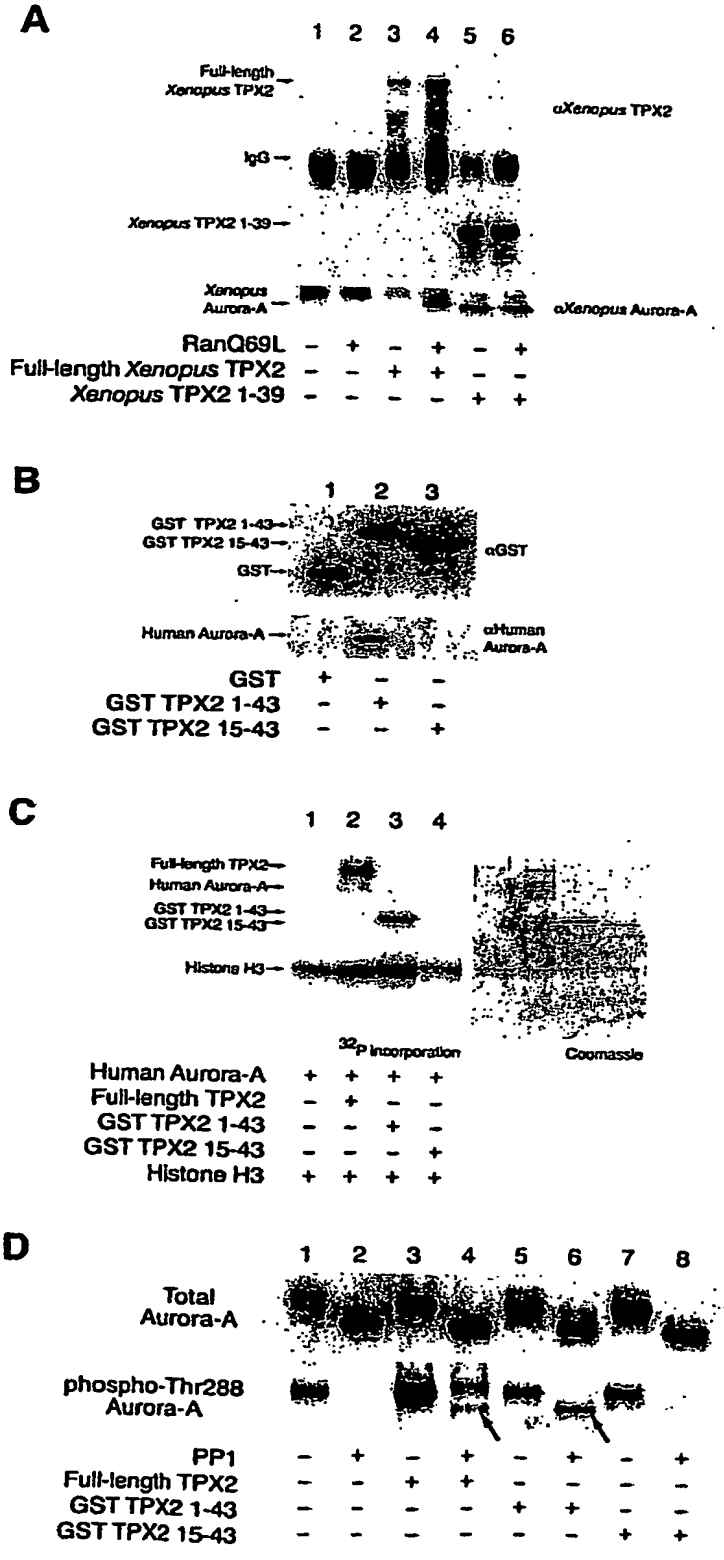


Fig. 2

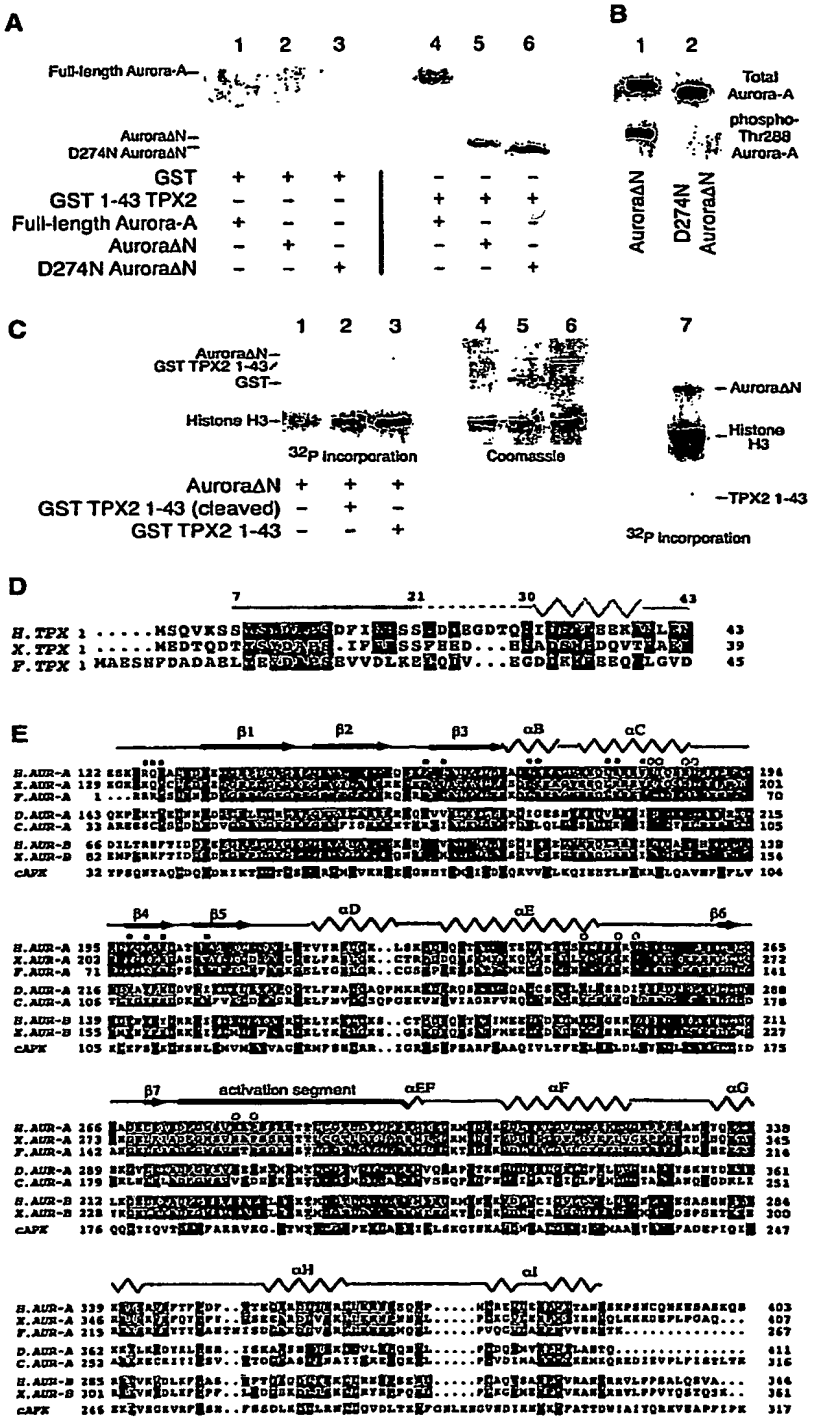


Fig. 3

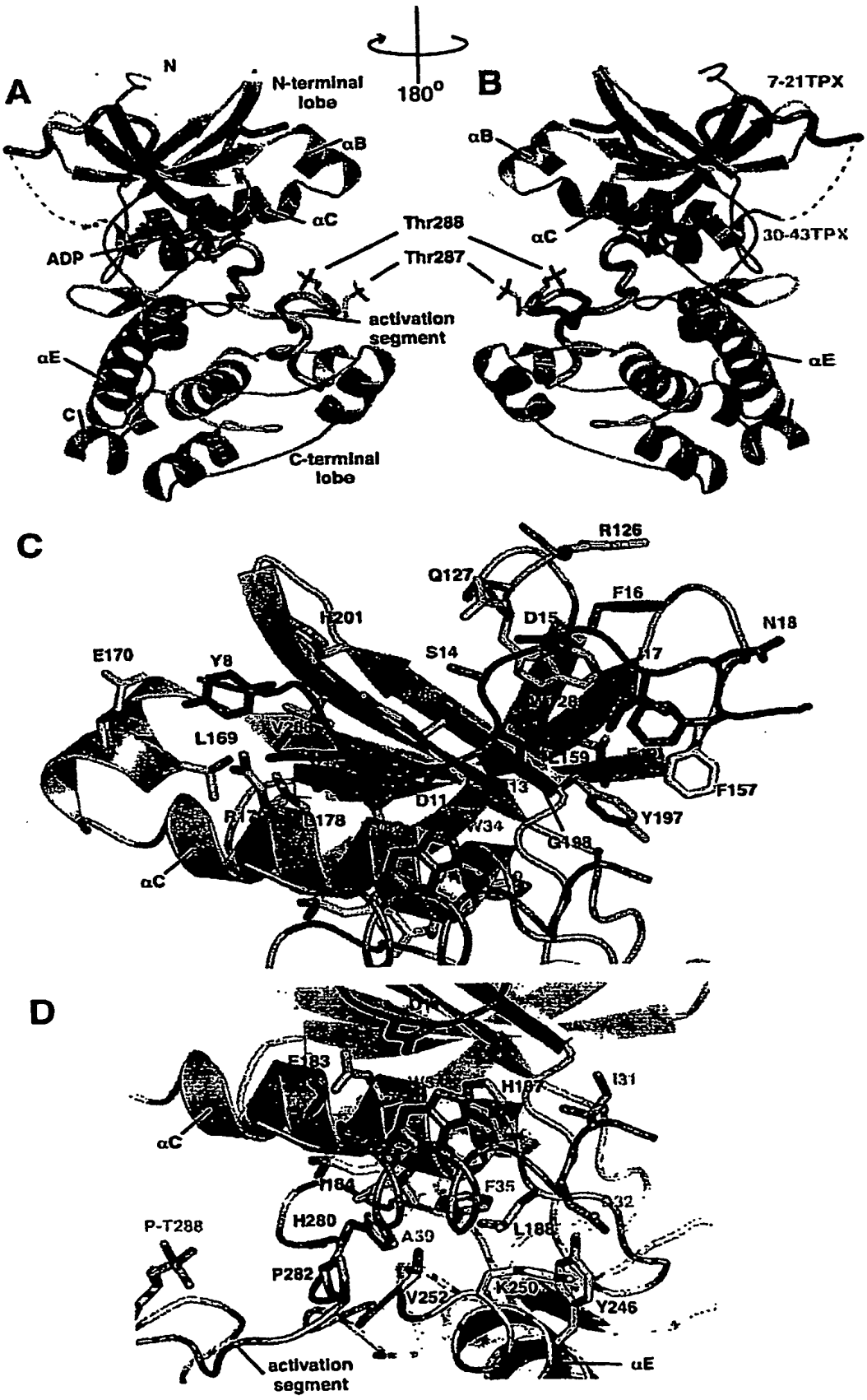


Fig. 4